



# The 24<sup>th</sup> International Annual Symposium on Computational Science and Engineering

## Confronting the Global Challenges

**Online by Cisco Webex Application,**

**Faculty of Liberal Arts and Science,  
Kasetsart University,  
Kamphaeng Saen campus, Nakhon Pathom, Thailand**

**April 28-30, 2021.**

**Co-organized and Sponsored by**



สมาคมวิชาการและวิศวกรรมเชิงคอมพิวเตอร์  
COMPUTATIONAL SCIENCE AND ENGINEERING ASSOCIATION



NATIONAL e-SCIENCE  
INFRASTRUCTURE CONSORTIUM





**Photo Credit:** *International Affairs, Public Relations and Community Relations  
Kasetsart University, Kamphaeng Saen Campus, Nakhon Pathom, Thailand.*



## WELCOME MESSAGE

**Assoc.Prof. Anuchai Pinyopummin, DVM, Ph.D.**  
 Vice President for Kasetsart University, Kamphaeng Saen Campus

Dear Colleagues, Professors, Lecturers and Researchers,

On behalf of Kasetsart University, Kamphaeng Saen Campus, It is my great pleasure to welcome you to the 24st International Annual Symposium on Computational Science and Engineering or ANSCSE24, which serves as an international forum for computational scientists and engineers. This symposium is also one of the largest gathering of Thai computational research community.

As you are aware, digital and online innovation are among the fastest growing technologies, which highly impact on the whole world in every aspects, especially in this “new normal” era. Here in Kasetsart University, Kamphaeng Saen Campus (KU.KPS), we provide research-based education with internationally recognized excellence in natural sciences. We also realize the important of computational science and its related filed as we have seen many signs of progress and so many interesting research being conducted in this area. For example, artificial intelligence and big data for material development, and advanced cloud computing technologies. Thus, we cannot deny the vital role that computational science plays in global research.

For this reason, we believe that ANSCSE24 under the theme of “Confronting the global challenges” ties well with this emerging digital era. In so doing, we believe that this symposium will provide opportunities for researchers and scholars from private sectors, academia, and research institutes in the field of computational science and engineering to exchange technical information, stimulate ideas and foster collaboration for driving sustainable innovation and economy.

We do hope that you have a fruitful time and enjoy not only the technical programs but also an effective online discussion. Thank you for your participation.

Sincerely yours,

**Assoc.Prof. Anuchai Pinyopummin, DVM, Ph.D.**

*Vice President for Kasetsart University,  
 Kamphaeng Saen Campus*



Dear Colleagues,

On behalf of Faculty of liberal arts and science, Kasetsart University, Kamphaeng Saen Campus, I am honored and delighted to welcome you to the 24<sup>th</sup> International Annual Symposium on Computational Science and Engineering (ANSCSE24). It is a great pleasure for our faculty to be the host of this symposium. Our co-hosts includes Computational Science and engineering Association (CSEA) and National e-Science Infrastructure Consortium; National Nanotechnology center (NANOTEC); and National Electronics and Computer Technology center (NECTEC).

Faculty of liberal arts and science was established in 1986. Over 28 years, our faculty has been developed continuously with 14 internal departments, over 9,000 students and 400 faculty staff. Our main mission is to provide teaching and learning on both social sciences and natural sciences to students. Also, one of our goals is to build academic alliances with other international institutions.

So, it is a great pleasure for us today, to organize this international symposium which has a long history of gathering researchers who are in the field of computational science and engineering to cross-fertilize ideas and to strengthen both local and international networks in computing science.

As the dean of Faculty of liberal arts and science, I would like to express my sincere appreciation to the steering committee, the honorary chairs, the international advisory board, the scientific chairs and committee, the reviewers, our sponsors and our organizing team, who has really worked hard in preparing all the technical programs and supporting other.

Finally, we hope that ANSCSE24 will truly serves the venue for networking and knowledge sharing among the participants which is an outcome of the comprehensive presentations as well as high-level plenary and panel sessions. We also hope that you will take utmost advantage of this event to start your future collaboration.

Sincerely yours,

**Assist. Prof. Dr. Anamai Damnet**

*Dean of Faculty of Liberal Arts and Science,  
Kasetsart University, Kamphaeng Saen Campus*



## WELCOME MESSAGE

**Dr. Varangkana Jitchum**

Head of Chemistry Division, Faculty of Liberal Arts and Science,  
Kasetsart University, Kamphaeng Saen Campus

Dear Colleagues,

It is a great pleasure and an honor to extend to you a warm welcome to attend the 24th International Annual Symposium on Computational Science and Engineering, or ANSCSE24. On behalf of Chemistry division, Faculty of Liberal Arts and Science, Kasetsart University, Kamphaeng Saen Campus, we are glad to be the main host for this international symposium.

The chemistry division was established in 1996. Since then, we have been providing the fundamentals of chemistry for undergraduate students across the campus. For more than a decade, our division has also committed to support advanced research in chemistry and materials in both experimental and computational area.

This year we are happy in organizing the ANSCSE24 which is one of the greatest gatherings of international computational scientists, computer science, and engineering researchers. I would like to thank our symposium staffs and also our co-host in jointly organizing this online symposium. Our partners are Computational Science and Engineering Association (CSEA), National Nanotechnology Center (NANOTEC), National Electronics and Computer Technology center (NECTEC), Chulalongkorn university, Mahidol university, Chiang mai university, Ubon ratchathani university, khon kaen university, Mahasarakham university, King Mongkut's University of Technology Thonburi, King Mongkut's University of Technology North Bangkok and National e-Science Infrastructure Consortium. We would like to acknowledge the Thai Journal of Mathematics indexed by Scopus, Computational and the Mathematical Methods (Wiley), Journal of Science and Science Education and Journal of Science and Science Education for supporting this symposium.

The online ANSCSE24 has been planned and divided in to 5 sessions depending on computational research criteria. Researchers who are taking part in this event are from both international and local academic institutions, and research organizations. The online symposium aims for the participants to share their experiences through the live stream presentations and discussion.

We hope ANSCSE24 will be an efficiency platform for you to discuss your ideas and strengthen connections with other researchers in the field. Last but not least, I would like to express my heartfelt thanks to the plenary speakers, invited speakers in each session, who are in their busy schedule but kindly manage their times to deliver highly stimulating talks for us in this symposium.

Sincerely yours,

**Dr. Varangkana Jitchum**

Head of Chemistry Division,  
Faculty of Liberal Arts and Science,  
Kasetsart University, Kamphaeng Saen Campus





Dear Friends and Colleagues,

On behalf of the Computational Science and Engineering Association (or in short CSEA), I am honored and delighted to welcome all of you to ANSCSE24 conference. It is a great honor for CSEA to be a co-host of ANSCSE24 together with Department of Chemistry, Faculty of liberal art and science, Kasetsart University, Kamphaengsaen Campus this year.

Over twenty years, ANSCSE has a long history of gathering researchers who are in the field of computational science and engineering to cross-fertilize ideas and to strengthen both local and international networks. Due to the covid19 pandemic, we could not hold the conference last year and we postponed it to this year. This is the first time we will make the ANSCSE conference online. The theme of this year is "Confronting the global challenges" Under this theme, ANSCSE24 covers various disciplines of computational science and engineering including fields of Chemistry, Physics, Biology, Fluid Dynamics, Solid Mechanics, High Performance Computing, Cloud Computing and Computer Science and Engineering.

This symposium aims to provide an exciting venue for scientists to present and exchange ideas, as well as to renew existing collaborations and to develop new ones. ANSCSE24 also offers a great opportunity for academic and industrial researchers to meet up and exchange ideas and information.

As the chair of CSEA, I would like to express my appreciation to all the committee chairs, the program chairs, the scientific committee, the reviewers, our sponsors, and especially the conference chair, Assistant Professor Bundet Boekfa. Last but not least; we should especially thank the local organizing committee teams. They have worked extremely hard in planning and organizing the technical programs and supporting the social arrangements.

Finally, ANSCSE24 truly serves as a venue for networking and knowledge sharing through comprehensive presentations as well as high-level plenary and panel sessions. We hope that everyone will gain new knowledge and think up of informative ideas for solving the global challenges ahead of us.

Sincerely yours,

**Dr. Supawadee Namuangruk**

President of Computational Science and Engineering Association  
(CSEA), Thailand

## COMMITTEES

### Steering Committee

- Prof. Vudhichai Parasuk Chulalongkorn University, Thailand
- Asst. Prof. Putchong Uthayopas Kasetsart University, Thailand
- Prof. Supa Hannongbua Kasetsart University, Thailand
- Assoc. Prof. Waraporn Parasuk Kasetsart University, Thailand
- Dr. Piyawut Srichaikul National Electronics and Computer Technology Center (NECTEC) Thailand

### Computational Chemistry Program Chair

- Dr. Supawadee Namuangruk National Nanotechnology Center (NANOTEC), NSTDA, Thailand
- Dr. Supareak Praserttham Chulalongkorn University, Thailand
- Assoc. Prof. Panida Surawatanawong Mahidol University, Thailand
- Dr. Pemika Srifa Kasetsart University, Thailand

### Computational Biology and Bioinformatics Program Chair

- Asst. Prof. Thanyada Rungrotmongkol Chulalongkorn University, Thailand
- Asst. Prof. Nadtanet Nunthaboot Mahasarakham University, Thailand
- Asst. Prof. Kamontip Kattiyawong Kasetsart University, Thailand

### Computational Physics, Computational Fluid Dynamics and Solid Mechanics Program Chair

- Assoc. Prof. Theerapong Puangmali Khon Kaen University, Thailand
- Asst. Prof. Piti Treesakul Kasetsart University, Thailand

### High Performance Computing, Computer Science, and Engineering Program Chair

- Dr. Manaschai Kunaseth National Electronics and Computer Technology Center (NECTEC), NSTDA, Thailand

### Mathematics and Statistic Program Chair

- Prof. Poom Kumam King Mongkut's University of Technology Thonburi, Thailand
- Prof. Phatiphat ThounThong King Mongkut's University of Technology North Bangkok, Thailand

## International Scientific Committee

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|--|--|
| <ul style="list-style-type: none"><li>• Prof. Michael Probst</li><li>• Prof. Joseph Samec</li><li>• Prof. Deva Priyakumar</li></ul>  | <ul style="list-style-type: none"><li>• University of Innsbruck, Austria</li><li>• Stockholm University, Sweden</li><li>• International Institute of Information Technology, India</li></ul>   |
| <ul style="list-style-type: none"><li>• Dr. Nongnuch Artrith</li><li>• Prof. Phornphimon Maitarad</li><li>• Prof. Maezono Ryo</li></ul>  | <ul style="list-style-type: none"><li>• Columbia University, USA</li><li>• Shanghai University, China</li><li>• Japan Advanced Institute of Science and Technology (JAIST), Japan</li></ul>  |
| <ul style="list-style-type: none"><li>• Prof. Hongo Kenta</li></ul>  | <ul style="list-style-type: none"><li>• Japan Advanced Institute of Science and Technology (JAIST), Japan</li></ul>  |
| <ul style="list-style-type: none"><li>• Prof. Kosuke Nakano</li></ul>  | <ul style="list-style-type: none"><li>• Japan Advanced Institute of Science and Technology (JAIST), Japan</li></ul>  |
| <ul style="list-style-type: none"><li>• Prof. Momoji Kubo</li><li>• Prof. Nobuki Ozawa</li><li>• Prof. Yusuke Ootani</li><li>• Prof. Emiel J. M. Hensen</li></ul>                                  | <ul style="list-style-type: none"><li>• Tohoku University, Japan</li><li>• Tohoku University, Japan</li><li>• Tohoku University, Japan</li><li>• Eindhoven University of Technology, Netherlands</li></ul>   |
| <ul style="list-style-type: none"><li>• Prof. Ivo Filot</li></ul>  | <ul style="list-style-type: none"><li>• Eindhoven University of Technology, Netherlands</li></ul>  |
| <ul style="list-style-type: none"><li>• Prof. Wolfgang Sippl</li></ul>   | <ul style="list-style-type: none"><li>• Institute of Pharmacy Martin-Luther-Universitaet Halle-Wittenberg, Germany</li></ul>   |
| <ul style="list-style-type: none"><li>• Prof. Yasuteru Shigeta</li><li>• Prof. Alessio Lodola</li><li>• Prof. Takahide Yamaguchi</li></ul>   | <ul style="list-style-type: none"><li>• University of Tsukuba, Japan</li><li>• Università di Parma, Italy</li><li>• National Institute for Materials Science, Japan</li></ul>  |
| <ul style="list-style-type: none"><li>• Prof. Ken-ichi Nomura</li><li>• Prof. Chris Lorenz</li><li>• Prof. Tiffany Walsh</li><li>• Prof. Ovidiu Bagdasar</li><li>• Prof. Damien Guilbert</li></ul> | <ul style="list-style-type: none"><li>• USC University of Southern California, USA</li><li>• King's College London, United Kingdom</li><li>• Deakin University, Australia</li><li>• University of Derby, United Kingdom</li><li>• Université de Lorraine, France</li></ul> |



## National Scientific Committee

- |                                       |   |
|---------------------------------------|---|
| • Dr. Supawadee Namuangruk            | National Nanotechnology Center<br>(NANOTEC), NSTDA, Thailand                        |
| • Assoc. Prof. Nawee Kungwan          | Chiang Mai University, Thailand   |
| • Prof. Siriporn Jungsuttiwong        | Ubon Ratchathani University, Thailand   |
| • Dr. Supareak Praserttham            | Chulalongkorn University, Thailand  |
| • Assoc. Prof. Panida Surawatanawong  | Mahidol University, Thailand  |
| • Asst. Prof. Thanyada Rungrotmongkol | Chulalongkorn University, Thailand  |
| • Asst. Prof. Nadtanet Nunthaboot     | Maharakham University, Thailand   |
| • Assoc. Prof. Theerapong Puangmali   | Khon Kaen University, Thailand  |
| • Dr. Manaschai Kunaseth              | National Electronics and Computer<br>Technology Center (NECTEC), NSTDA,<br>Thailand |
| • Prof. Poom Kumam                    | King Mongkut's University of Technology<br>Thonburi, Thailand                       |
| • Prof. Phatiphat ThounThong          | King Mongkut's University of Technology<br>North Bangkok, Thailand                  |
| • Prof. Rachata Ausavarungrun         | King Mongkut's University of Technology<br>North Bangkok, Thailand                  |
| • Assoc. Prof. Watshara Shoombuatong  | Mahidol University, Thailand  |
| • Assoc. Prof. Taweetham Limpanuparb  | Mahidol University, Thailand  |
| • Asst. Prof. Thana Sutthibutpong     | King Mongkut's University of Technology<br>Thonburi, Thailand                       |
| • Assoc. Prof. Usa Humphries          | King Mongkut's University of Technology<br>Thonburi, Thailand                       |
| • Asst. Prof. Bundet Boekfa           | Kasetsart University, Thailand  |
| • Dr. Thana Maihom                    | Kasetsart University, Thailand  |

## Organizing Committee Chair

- |                             |                                |
|-----------------------------|--------------------------------|
| • Asst. Prof. Bundet Boekfa | Kasetsart University, Thailand |
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## Organizing Committee

- |  |  |
|--|--|
| • Dr. Supawadee Namuangruk             | National Nanotechnology Center<br>(NANOTEC), NSTDA, Thailand |
| • Assoc. Prof. Nawee Kungwan           | Chiang Mai University, Thailand                              |
| • Prof. Siriporn Jungsuttiwong         | Ubon Ratchathani University, Thailand                        |
| • Asst. Prof. Thanyada Rungrotmongkol  | Chulalongkorn University, Thailand                           |
| • Asst. Prof. Anamai Damnet            | Kasetsart University, Thailand                               |
| • Dr. Varangkana Jitchum               | Kasetsart University, Thailand                               |
| • Asst. Prof. Bundet Boekfa            | Kasetsart University, Thailand                               |
| • Asst. Prof. Piti Treesukol           | Kasetsart University, Thailand                               |
| • Asst. Prof. Arthorn Loisruangsin     | Kasetsart University, Thailand                               |
| • Asst. Prof. Kamontip Kuttiyawong     | Kasetsart University, Thailand                               |
| • Asst. Prof. Sunan Tiptipakorn        | Kasetsart University, Thailand                               |
| • Asst. Prof. Namfon Tongtavee         | Kasetsart University, Thailand                               |
| • Asst. Prof. Potjaman Poolmee         | Kasetsart University, Thailand                               |
| • Asst. Prof. Sasiwadee Boonya-udtayan | Kasetsart University, Thailand                               |
| • Asst. Prof. Thitiya Pung             | Kasetsart University, Thailand                               |
| • Asst. Prof. Veeramol Vailikhit       | Kasetsart University, Thailand                               |
| • Asst. Prof. Weenawan Somphon         | Kasetsart University, Thailand                               |
| • Dr. Thana Maihom                     | Kasetsart University, Thailand                               |
| • Dr. Nongpanga Jarussophon            | Kasetsart University, Thailand                               |
| • Dr. Nuanjan Matchariyakul            | Kasetsart University, Thailand                               |
| • Dr. Songtham Ruangchaithaweesuk      | Kasetsart University, Thailand                               |
| • Dr. Tipawan Rungsawang               | Kasetsart University, Thailand                               |
| • Dr. Pemika Srifa                     | Kasetsart University, Thailand                               |
| • Dr. Wanpen Laosripaiboon             | Kasetsart University, Thailand                               |
| • Ms. Wilailuck Kwangyuen              | Kasetsart University, Thailand                               |

## SESSION SUMMARY

### Plenary Lecture

- PL-1** Prof. Dr. Michael Probst  
University of Innsbruck, Austria
- PL-2** Prof. Dr. Joseph Samec  
Stockholm University, Sweden
- PL-3** Dr. Nongnuch Artrith  
Columbia University, USA
- PL-4** Prof. Dr. Deva Priyakumar  
International Institute of Information Technology, India

### Scientific Session

ANSCSE24 will be held under the theme “Confronting the Global Challenges” and will cover topics in the following

- CHE** Computational Chemistry
- PFD** Computational Physics, Computational Fluid Dynamics, and Solid Mechanics
- BIO** Computational Biology, Bioinformatics, Biochemistry, and Biophysics
- CSE** High Performance Computing, Computer Science, and Engineering
- MST** Mathematics and Statistics

# OVERALL PROGRAM

**Wednesday, 28 April 2021**

Thailand Time	
8:00-8:30	Online Registration
8:30-10:20	<b>Opening Ceremony</b>
10:20-10:30	Break
10:30-12:10	Two Parallel Sessions
10:30-11:10	<b>CHE</b>
11:10-11:40	(CHE-I-01) Prof. Ryo Maezono (40 min) <i>Japan Advanced Institute of Science and Technology</i> (Japan Time 12.30-13.10)
11:40-12:10	(CHE-I-02) Prof. Kenta Hongo (30 min) <i>Japan Advanced Institute of Science and Technology</i> (Japan Time 13.10-13.40)
	(CHE-I-03) Prof. Kosuke Nakano (30 min) <i>Japan Advanced Institute of Science and Technology</i> (Japan Time 13.40-14.10)
	<b>PFD</b>
	(PFD-I-01) Prof. Tiffany Walsh (40 min) <i>Deakin University, Australia</i> (Australia Time 13.30-14.10)
	Contributed speakers (15 min/person) (PFD-O-01), (PFD-O-02), (PFD-O-03), (PFD-O-04)
12:10-13:00	Lunch Break
13:00-14:40	Two Parallel Sessions
13:00-13:40	<b>CHE</b>
13:40-14:10	(CHE-I-04) Prof. Momiji Kubo (40 min) <i>Tohoku University</i> (Japan Time 15.00-15.40)
14:10-14:40	(CHE-I-05) Prof. Nobuki Ozawa (30 min) <i>Tohoku University</i> (Japan Time 15.40-16.10)
	(CHE-I-06) Prof. Yusuke Ootani (30 min) <i>Tohoku University</i> (Japan Time 16.10-16.40)
	<b>PFD</b>
	(PFD-I-02) Prof. Thana Sutthibutpong (40 min)(KMUTT, Thailand)
	Contributed speakers (15 min/person) (PFD-O-05), (PFD-O-06), (PFD-O-07), (PFD-O-08)
14:40-14:50	Break
<b>Chairman: Dr. Supawadee Namuangruk; Co-chairman: Dr. Pemika Srifa</b>	
14:50-15:30	<b>Plenary</b> - Prof. Dr. Michael Probst (40 min) <i>University of Innsbruck, Austria</i> (Austria Time 9.50-10.30)
15:30-16:10	<b>Plenary</b> - Prof. Dr. Joseph Samec (40 min) <i>Stockholm University, Sweden</i> (Sweden Time 10.30-11.10)
16:10-18:00	Two Parallel Sessions
16:10-16:50	<b>CHE</b>
16:50-17:20	(CHE-I-07) Prof. Emiel J.M. Hensen (40 min) <i>Eindhoven University of Technology</i> (Netherlands Time 11.10-11.50)
	(CHE-I-08) Prof. Ivo Filot (30 min) <i>Eindhoven University of Technology</i> (Netherlands Time 11.50-12.20)
	<b>PFD</b>
	(PFD-I-03) Prof. Chris Lorenz (40 min) <i>King's College London, United Kingdom</i> (United Kingdom Time 10.10-11.00)
	Contributed speakers (15 min/person) (PFD-O-09)
17:20-17:30	Break
17:30-18:30	Contributed speakers (15 min/person) (CHE-O-01), (CHE-O-02), (CHE-O-03), (CHE-O-04)

**Thursday, 29 April 2021**

<b>Thailand Time</b>	
<b>Chairman:</b> Prof. Siriporn Jungsuttiwong; <b>Co-chairman:</b> Asst. Prof. Bundet Boekfa	
8:30-9:10	<b>Plenary</b> - Dr. Nongnuch Artrith (40 min) <i>Columbia University, USA</i> (New York Time 21.30-22.10 on April 28)
9:20-10:00	<b>Plenary</b> - Prof. Dr. Deva Priyakumar (40 min) <i>International Institute of Information Technology, India</i> (India Time 7.40-8.10)
10:00-10:10	<b>Break</b>
<b>10:10-12:10</b>	<b>Two Parallel Sessions</b>
10:10-10:40	<b>CHE</b>
10:40-11:10	(CHE-I-09) Assoc.Prof. Taweetham Limpanuparb (30 min) <i>Mahidol University International College (MUIC)</i>
11:10-11:40	(CHE-I-10) Dr. Supareak Praserttham (30 min) <i>Chulalongkorn University</i>
11:40-12:10	(CHE-O-05) Prof. Tim Kowalczyk (30 min) <i>Western Washington University</i> (USA, Seattle Time 21.10-21.40 on April 28)
	(CHE-I-11) Prof. Jitrayut Jitonnorn (30 min) <i>Phayao University</i>
12:10-13:00	<b>Lunch Break</b>
<b>13:00-14:40</b>	<b>Two Parallel Sessions</b>
13:00-14:40	<b>BIO</b>
	(BIO-I-01) Prof. Wolfgang Sippl (40minutes) <i>Martin-Luther-Universitaet Halle-Wittenberg</i> (German Time 8.00-8.40)
	Contributed speakers (15 min/person) (BIO-O-01), (BIO-O-02) (BIO-O-03), (BIO-O-04)
	<b>MST</b>
	(MST-I-02) Prof. Ovidiu Bagdasar (30 min) <i>University of Derby, UK</i> (UK Time 7.00-7.30)
	(MST-I-03) Prof.Damien Guilbert (30 min) <i>Université de Lorraine, France</i> (France Time 8.30-9.00)
	MST: 3 Speakers (15 min/person) (MST-O-07), (MST-O-08), (MST-O-09)
14:40-15:00	<b>Break</b>
<b>15:00-18:00</b>	<b>POSTER (CHE + BIO + PFD)</b> (5 min/person) CHE-P-01-15, BIO-P-01-06, PHYS-P-01-03
15:00-16:30	MST: 4 Speakers (15 min/person) (MST-O-10), (MST-O-11), (MST-O-12), (MST-O-13), (MST-O-14), (MST-O-15)
16:30-16:40	<b>Break</b>
16:40-17:40	<b>POSTER (CHE + BIO + PFD)</b> (5 min/person) CHE-P-01-15, BIO-P-01-06, PHYS-P-01-03
	MST: 4 Speakers (15 min/person) (MST-O-16), (MST-O-17) (MST-O-18), (MST-O-19), (MST-O-20)

**Friday 30 April 2021**

Time		
<b>9:00-10:20</b>	Two Parallel Sessions	
9:00-9:30	<b>BIO</b>	<b>CSE</b>
9:30-10:00	(BIO-I-02) Prof. Yasuteru Shigeta (30 min) <i>University of Tsukuba</i> (Japan Time 11.00-11.30)	(CSE-I-01) Prof. Ken-ichi Nomura (30 min) <i>USC, USA</i> (California Time 19.00-19.30 on April 29)
10:00-10:30	(BIO-I-03) Prof. Takahide Yamaguchi (30 min) <i>Ibaraki University</i> (Japan Time 11.30-12.00)	(CSE-I-02) Prof. Rachata Ausavarungrun (30 mins) <i>KMUTNB</i> (CSE-I-03) Dr. Sakda Tridech (30 min) <i>Pollution Control Department</i>
	Contributed speakers (15 min/person) (BIO-O-05), (BIO-O-06)	
<b>10:30-10:40</b>	Break	
10:40-11:10	(BIO-I-04) Prof. Watshara Shoombuatong (30 min) <i>Mahidol University</i>	CSE: 5 Speakers (15 min/person) (CSE-O-01), (CSE-O-02), (CSE-O-03), (CSE-O-04), (CSE-O-05)
11:10- 12:00	Contributed speakers (15 min/person) (BIO-O-07) (BIO-O-09)	
<b>12:00-13:00</b>	Lunch Break	
13:00-13:30	<b>BIO</b>	<b>MST</b>
	(BIO-I-05) Prof. Alessio Lodola (30 min) <i>Università di Parma, Italy</i> (Italy Time 8.00-8.30)	MST: 4 Speakers (15 min/person) (MST-O-21), (MST-O-22), (MST-O-23), (MST-O-24)
13:30-14:00	Contributed speakers (15 min/person) (BIO-O-10) (BIO-O-11)	
<b>14:00-14:10</b>	Break	
14:10-14:50	Contributed speakers (15 min/person) (BIO-O-12) (BIO-O-13)	MST: 2 Speakers (15 min/person) (MST-O-25), (MST-O-26) (MST-O-27)
<b>14:50-16:00</b>	Break	
16:00-16:30	Closing Conference : Award Announcements	

## SCIENTIFIC PROGRAM

**Session:** Computational Chemistry (CHE)

<b>Wednesday, April 28, 2021</b>	
<b>Chairman:</b> Dr. Supareak Prasertthdam; Co-chairman: Dr. Thana Maihom	
10:30-11:10	CHE-I-01: Prof. Ryo Maezono
11:10-11:40	CHE-I-02: Prof. Kenta Hongo
11:40-12:10	CHE-I-03: Prof. Kosuke Nakano
12:10-13:00	Lunch
<b>Chairman:</b> Dr. Supareak Prasertthdam; Co-chairman: Dr. Thana Maihom	
13:00-13:40	CHE-I-04: Prof. Momoji Kubo
13:40-14:10	CHE-I-05: Prof. Nobuki Ozawa
14:10-14:40	CHE-I-06: Prof. Yusuke Ootani
14:40-14:50	Break
<b>Chairman:</b> Dr. Supareak Prasertthdam; Co-chairman: Dr. Thana Maihom	
16:10-16:50	CHE-I-07: Prof. Emiel J.M. Hensen
16:50-17:20	CHE-I-08: Prof. Ivo Filot
17:20-17:30	Break
<b>Chairman:</b> Dr. Supawadee Namuangruk; Co-chairman: Dr. Thana Maihom	
17:30-17:45	CHE-O-01: Fadjar Mulya
17:45-18:00	CHE-O-02: Phakawan Thinsoongnoen
18:00-18:15	CHE-O-03: Suparada Kamchompoo
18:15-18:30	CHE-O-04: Nutchanon Somwatcharajit

<b>Thursday, April 29, 2021</b>	
<b>Chairman:</b> Assoc. Prof. Panida Surawatanawong; Co-chairman: Asst. Prof. Thitiya Pung	
10:10-10:40	CHE-I-09: Assoc. Prof. Taweetham Limpanuparb
10:40-11:10	CHE-I-10: Dr. Supareak Prasertthdam
11:10-11:40	CHE-O-05: Assoc. Prof. Tim Kowalczyk
11:40-12:10	CHE-I-11: Assoc. Prof. Jitrayut Jitonnorn
12:10-13:00	Lunch
15:00-18:30	<b>Poster Session</b>



**Session:** Computational Physics, Computational Fluid Dynamics and Solid Mechanics (PFD)

<b>Wednesday, April 28, 2021</b>	
<b>Chairman:</b> Assoc. Prof. Theerapong Puangmali; Co-chairman: Asst. Prof. Piti Treesukol	
10:30-11:10	PFD-I-02: Prof. Tiffany Walsh
11:10-11:25	PFD-O-01: Chananun Rojanarungruengporn
11:25-11:40	PFD-O-02: Auwalu Hamisu Usman
11:40-11:55	PFD-O-03: Nutnicha Naknual
11:55-12:10	PFD-O-04: Sataporn Kala
12:10-13:00	Lunch
<b>Chairman:</b> Assoc. Prof. Theerapong Puangmali; Co-chairman: Asst. Prof. Weenawan Somphon	
13:00-13:40	PFD-I-03: Prof. Thana Sutthibutpong
13:40-13:55	PFD-O-05: Unnop Srikulwong
13:55-14:10	PFD-O-06: Chanadan Douykhumklaw
14:10-14:25	PFD-O-07: Talha Anwar
14:25-14:40	PFD-O-08: Asifa
14:40-14:50	Break
<b>Chairman:</b> Assoc. Prof. Theerapong Puangmali; Co-chairman: Asst. Prof. Weenawan Somphon	
16:10-16:50	PFD-I-01: Prof. Chris Lorenz
16:50-17:05	PFD-O-09: Nachat Jatusripitak

**Session: Computational Biology, Bioinformatics, Biochemistry, and Biophysics (BIO)**

<b>Thursday, April 29, 2021</b>	
<b>Chairman:</b> Asst. Prof. Nadtanet Nunthaboot; <b>Co-chairman:</b> Asst. Prof. Kamontip Kuttiyawong	
13:00-13:40	BIO-I-01: Prof. Wolfgang Sippl
13:40-13:55	BIO-O-01: Dr. Wittaya Pheera
13:55-14:10	BIO-O-02: Chonnikan Hanpaibool
14:10-14:25	BIO-O-03: Noppavit Kaewlin
14:25-14:40	BIO-O-04: Nawanwat C. Pattarangoon
14:40-15:00	Break
15:00-18:00	Poster Session

<b>Friday, April 30, 2021</b>	
<b>Chairman:</b> Asst. Prof. Thanyada Rungrotmongkol; <b>Co-chairman:</b> Asst. Prof. Sunan Tiptipakorn	
9:00-9:30	BIO-I-02: Prof. Yasuteru Shigeta
9:30-10:00	BIO-I-03: Prof. Takahide Yamaguchi
10:00-10:15	BIO-O-05: Dr. Kanyani Sangphak
10:15-10:30	BIO-O-06: Nayana Bhat
10:30-10:40	Break
<b>Chairman:</b> Asst. Prof. Nadtanet Nunthaboot; <b>Co-chairman:</b> Asst. Prof. Kamontip Kuttiyawong	
10:40-11:10	BIO-I-04: Prof. Watshara Shoombuatong
11:10-11:25	BIO-O-07: Pitchayathida Mee-udorn
11:25-11:40	<del>BIO-O-08:</del>
11:40-11:55	BIO-O-09: Nitchakan Darai
12:00-13:00	Lunch
<b>Chairman:</b> Asst. Prof. Thanyada Rungrotmongkol; <b>Co-chairman:</b> Asst. Prof. Sunan Tiptipakorn	
13:00-13:30	BIO-I-05: Prof. Alessio Lodola
13:30-13:45	BIO-O-10: Hathaichanok Chuntakaruk
13:45-14:00	BIO-O-11: Witthawat Phanchai
14:00-14:10	Break
14:10-14:25	BIO-O-12: Kun Karnchanapandh
14:25-14:40	BIO-O-13: Amita Sripattaraphan

**Session:** High Performance Computing, Computer Science and Engineering (CSE)

<b>Friday, April 30, 2021</b>	
<b>Chairman:</b> Dr. Manaschai Kunaseth; Co-chairman: Asst. Prof. Arthorn Loisruangsin	
9:00-9:30	CSE-I-01: Prof. Ken-ichi Nomura
9:30-10:00	CSE-I-02: Prof. Rachata Ausavarungnirun
10:00-10:30	CSE-I-03: Dr. Sakda Tridech
10:30-10:40	Break
10:40-10:55	CSE-O-01: Dr. Putt Sakdhnagool
10:55-11:10	CSE-O-02: Dr. Aliyu Muhammed Awwal
11:10-11:25	CSE-O-03: Saknarin Channark
11:25-11:40	CSE-O-04: Sani Aji
11:40-11:55	CSE-O-05: Idris Ahmed
12:00-13:00	Lunch

**Session: Mathematics and Statistics (MST)**

<b>Thursday, April 29, 2021</b>	
<b>Chairman:</b> Prof. Poom Kumam; Prof. Phatiphat ThounThong; Assoc.Prof.Chirasak Mongkolkeha <b>Co-chairman:</b> Dr. Tipawan Rungsawang	
10:10-10:40	MST-I-01: Assoc. Prof. Usa Humphries
10:40-10:55	MST-O-01: Assoc. Prof. Chirasak Mongkolkeha
10:55-11:10	MST-O-02: Asst. Prof. Thidaporn Seangwattana
11:10-11:25	MST-O-03: Dr. Sabah Iftikhar
11:25-11:40	MST-O-04: Dr. Konrawut Khammahawong
11:40-11:55	MST-O-05: Kabin Kanjamapornkul
11:55-12:10	MST-O-06: Habib ur Rehman
12:10-13:00	Lunch
<b>Chairman:</b> Prof. Poom Kumam; Prof. Phatiphat ThounThong; Assoc.Prof.Chirasak Mongkolkeha <b>Co-chairman:</b> Asst. Prof. Potjaman Poolmee	
13:00-13:30	MST-I-02: Prof. Ovidiu Bagdasar
13:30-14:00	MST-I-03: Prof. Damien Guilbert
14:00-14:15	MST-O-07: Asst. Prof. Tanakit Thianwan
14:15-14:30	MST-O-08: Dr. Auwal Bala Abubakar
14:30-14:45	MST-O-09: Nagornchat Chansuriya
14:45-14:50	Break
<b>Chairman:</b> Prof. Poom Kumam; Prof. Phatiphat ThounThong; Assoc.Prof.Chirasak Mongkolkeha <b>Co-chairman:</b> Dr. Songtham Ruangchaithaweek	
15:00-15:15	MST-O-10: Dr. Ronnachai Nanthochot
15:15-15:30	MST-O-11: Dr. Ali Turab
15:30-15:45	MST-O-12: Dr. Thanatporn Bantaojai
15:45-16:00	MST-O-13: Dr. Piyachat Borisut
16:00-16:15	MST-O-14: Tanapon Khampichit
16:15-16:30	MST-O-15: Syed Irtaza Hassnain
16:30-16:40	Break
<b>Chairman:</b> Prof. Poom Kumam; Prof. Phatiphat ThounThong; Assoc.Prof.Chirasak Mongkolkeha <b>Co-chairman:</b> Dr.Songtham Ruangchaithaweek	
16:40-16:55	MST-O-16: Chonjaroen Chairatsiripong
16:55-17:10	MST-O-17: Apassara Suechoei
17:10-17:25	MST-O-18: Wachirapong Jirakitpuwapat
17:25-17:40	MST-O-19: Ponkamon Kitisak
17:40-17:55	MST-O-20: Pronpat Peeyada
<b>Friday, April 30, 2021</b>	
<b>Chairman:</b> Prof. Poom Kumam; Prof. Phatiphat ThounThong; <b>Co-chairman:</b> Asst. Prof. Piti Treesukol	
13:00-13:15	MST-O-21: Asst. Prof. Rungsarit Intaramo
13:15-13:30	MST-O-22: Dr. Muhammad Sohail
13:30-13:45	MST-O-23: Chaiwat Auipa-arch
13:45-14:00	MST-O-24: Suparat Kesornprom
14:00-14:10	Break
<b>Chairman:</b> Prof. Poom Kumam; Prof. Phatiphat ThounThong; <b>Co-chairman:</b> Asst. Prof. Piti Treesukol	
14:10-14:25	MST-O-25: Kunrada Kankam
14:25-14:40	MST-O-26: Kittisak Amnuaykarn
14:40-14:55	MST-O-27: Jarucha Puttharak

**Poster session PFD, BIO and CHE**

<b>Thursday, April 29, 2021</b>		
<b>Chairman:</b> Dr. Supawadee Namuangruk, Dr. Supareak Praserttham, Assoc. Prof. Panida Surawatanawong, Assoc. Prof. Theerapong Puangmali, Asst. Prof. Thanyada Rungrotmongkol, Asst. Prof. Nadtanet Nunthaboot; <b>Co-chairman:</b> Dr. Thana Maihom, Asst. Prof. Veeramol Vailikhit		
15:00-15:30	PFD-P-01 BIO-P-01 BIO-P-02 BIO-P-03	Assoc. Prof. Pairot Moontragoon Nikorn Shinsuphan Napat Kongtaworn Amy Oo
15.30-16.00	BIO-P-04 BIO-P-05 BIO-P-06 CHE-P-01	Duangjai Todsaporn Saowalak Somjid Utidi Suriya Dr. Teeranan Nongnual
16.00-16.30	CHE-P-02 CHE-P-03 CHE-P-04 CHE-P-05	Dr. Pornsawan Sikam Dr. Yutthana Wongnongwa Shokirbek Shermukhamedov Mookda Meechai
<b>Chairman:</b> Dr. Supawadee Namuangruk, Dr. Supareak Praserttham, Assoc. Prof. Panida Surawatanawong, Assoc. Prof. Theerapong Puangmali, Asst. Prof. Thanyada Rungrotmongkol, Asst. Prof. Nadtanet Nunthaboot; <b>Co-chairman:</b> Dr. Nongpanga Jarussophon, Asst. Prof. Bundet Boekfa		
16:40-17:10	CHE-P-06 CHE-P-07 CHE-P-08 CHE-P-09	Komkrit Anurak Yuwanda Injongkol Muhammad Dzulfahmi Ramadhan Krongkwan Nilwanna
17.10-17.40	CHE-P-10 CHE-P-11 CHE-P-12 CHE-P-13	Patraporn Srirattanasakunsuk Mattanun Sangkhawasi Munchalika Jaitrong Chirawat Chitpakdee
17.40-18.10	CHE-P-14 CHE-P-15 CHE-P-16 CHE-P-17	Thanadol Jitwatanasirikul Yodsri Nanakorn Kansuda Trisuwan Pimjai Pimboatham
18.10-18.40	CHE-P-18 KPS-P-01 KPS-P-02 KPS-P-03	Ratchadaree Intayot Chalarat Chaemchamrat Piyapha Cheamchoi Suphanni Jaichueai

## PLENARY LECTURES

# PL-1

## Machine Learning in Materials Science :Simulation of Surface Sputtering and General Considerations

**Michael Probst<sup>1a</sup>, Shermux. Shermukhamedov<sup>1</sup>, and Lei Chen<sup>1</sup>**

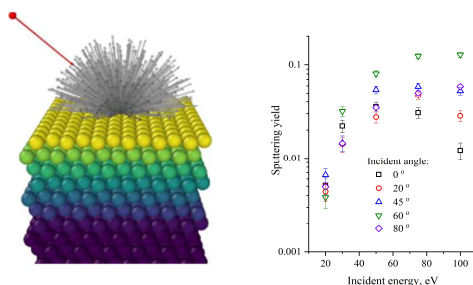
<sup>1</sup>*Institute of Ion Physics and Applied Physics, University of Innsbruck, Technikerstrasse 25, 6020 Innsbruck, Austria,*

<sup>a</sup>*E-mail: michael.probst@uibk.ac.at*

### ABSTRACT

**Keywords:** Computational Materials Science, Machine Learning, Molecular Dynamics Simulations

Techniques like machine learning, Bayesian inference and uncertainty quantification are increasingly used in science and engineering. We discuss some of them and give a material science example of using neural networks as potential energy functions: We study sputtering of surfaces, an important process in materials science. An example is beryllium sputtering by hydrogen isotopes [1], leading to surface damage which is vital to know in nuclear fusion materials. Sputtering involves many parameters: Material, surface temperature, impact energy and angle and so on. We model the sputtering by means of non-cumulative molecular dynamics simulations with a large number trajectories for each set of parameters. The forces and energies required are calculated by means of density functional calculations fitted to high-dimensional neural networks. After this example we discuss general guidelines in the ever-evolving discussion of data driven versus physics-driven modelling [2,3].



**Figure:** Left: Visualisation of incoming D and distribution of sputtered Be. Right: Sputtering rate as function of the kinetic energy for different incident angles.

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3. "White paper on gaps and obstacles in materials modelling", The European Materials Modelling Council, <https://emmc.info/wp-content/uploads/2019/12/EMMC-CSA-whitepaper-DRAFTV20191220v2.pdf>



**Prof. Michael Probst** received his PhD degree from Innsbruck University in 1983. Currently he is Professor at the Ion Physics Institute of Innsbruck University in Austria. His research interests focus on theoretical materials science, modelling, quantum chemistry and on applications of machine learning in physics and chemistry.



## PL-2

# Computational Chemistry: A Last Resort for the Bona Fide Experimentalist?

Joseph S. M. Samec <sup>1,2,\*</sup>

<sup>1</sup>Department of Organic Chemistry, Stockholm University, 10691 Stockholm, Sweden

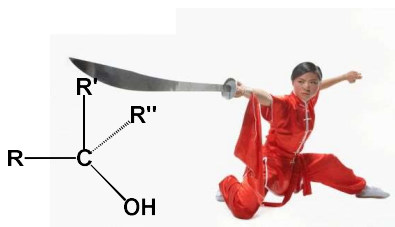
<sup>2</sup> Department of Chemistry, Chulalongkorn University, Pathumwan, Bangkok 10330, Thailand

\* E-mail: joseph.samec@su.se; Tel. +46 8 16 31 14

### ABSTRACT

**Keywords:** DFT, Experimental, Reaction Mechanism, Catalysis, Green Chemistry

The experimentalist has a diverse tool box to study the reaction mechanism of a transformation in chemistry. For example: isolating reactive intermediates, Hammet plots, isotopic labelling, designing substrates where a reactive position is blocked and kinetics including rate-order and kinetic isotope effect. However, sometimes the experimentalist cannot design an experiment to elucidate a critical step of a reaction. In such situations, the computational chemistry is not only a supplement to experiments, but a necessity to reach an understanding of fundamental steps in a reaction mechanism. Under this talk, an account covering four diverse examples of such situations will be disclosed. All examples include novel reactions in Green Chemistry, and the interaction between the substrate and the catalyst in critical key steps of the transformations often during a C-O bond cleaving event.



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**Prof. Joseph Samec** is professor in organic chemistry at Stockholm university working on biomass valorization. He is interested in both developing chemical methodologies as well as fundamental studies of the reaction mechanism. He has above 70 publications, 25 patents and founded 4 companies in biomass valorization

## PL-3 Modelling of Complex Energy Materials with Machine Learning

Nongnuch Artrith<sup>1\*</sup>

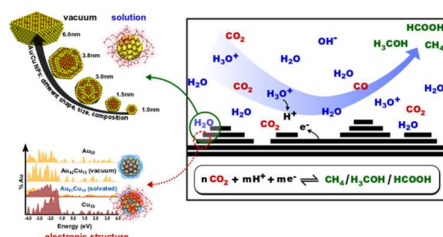
<sup>1</sup>Department of Chemical Engineering, and Columbia Center for Computational Electrochemistry, Columbia University, USA

\* E-mail: nartrith@atomistic.net; Tel. +18575238452

### ABSTRACT

**Keywords:** DFT, Machine Learning, Artificial Neural Networks, Energy Materials

The properties of materials for energy applications, such as heterogeneous catalysts and battery materials, often depend on complicated chemical compositions and complex structural features including defects and disorder. This complexity makes the direct modelling with first principles methods challenging. Machine-learning (ML) potentials trained on first principles reference data enable linear-scaling atomistic simulations with an accuracy that is close to the reference method at a fraction of the computational cost. ML models can also be trained to predict the outcome of simulations (or experiments), bypassing explicit atomistic modelling altogether. In this talk, I will give an overview of recent methodological advancements of ML potentials based on artificial neural networks (ANNs) [1-5] and applications of the method to challenging materials classes including metal and oxide nanoparticles and amorphous phases. Further, I will show an example of integrating large computational and small experimental data sets for the ML-guided discovery of catalyst materials [6].



**Figure 1** .Electrochemical Interfaces :Complex Systems are challenging for Simulations.

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**Nongnuch Artrith** received her PhD degree from Ruhr University Bochum, Germany, in 2013. Nongnuch is currently a Research Scientist at Columbia University, USA, after postdoctoral training at MIT and UC Berkeley. Her research interests focus on the development and application of first principles and machine-learning methods for the computational discovery of energy materials and for the interpretation of experimental observations.

## PL-4 Artificial Intelligence for Molecular Design

U. Deva Priyakumar\*

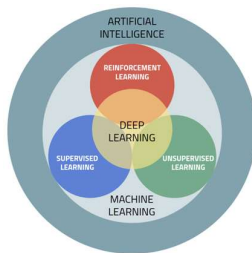
Center for Computational Natural Sciences and Bioinformatics, International Institute of Information Technology, Hyderabad 500 032, India

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### ABSTRACT

**Keywords:** Drug Design, Machine Learning, Deep Learning, Molecular Modeling

The area of molecular sciences witnessed the rise and fall of artificial intelligence (AI)/ machine learning (ML) methods, especially artificial neural networks, few decades ago. However, we see a major resurgence in the use of modern ML methods in scientific research during the recent years. These methods have had phenomenal success in the areas of computer vision, speech recognition, natural language processing (NLP), etc., which has inspired chemists and biologists to apply these algorithms to problems in natural sciences. Availability of high performance GPU-accelerators, data, new algorithms and libraries has enabled this surge. ML algorithms have successfully been applied to various domains in molecular sciences by providing much faster and accurate solutions compared to traditional methods like QM calculations, DFT or MM-based methods, etc. Some of the areas where the potential of ML methods has been shown to be effective are in drug design, prediction of high level quantum mechanical energies, molecular design, molecular dynamics and retrosynthesis of organic compounds. This presentation will discuss some of our attempts in the use of modern ML methods for molecular design.



**Figure 1.** Artificial Intelligence – Machine Learning – Deep Learning

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**U. Deva Priyakumar** is a Professor in International Institute of Information Technology, Hyderabad. His research interests involve application of computational methods to study chemical/biological systems and processes. Currently, his group is applying machine learning techniques for drug design and healthcare. He has been awarded such as the Chemical research society of India Medal (2021), Chemical Society of Japan distinguished lecture.

## **INVITED SPEAKERS**

# CHE-I-01

## Electronic structure calculation using Diffusion Monte Carlo methods

Ryo Maezono

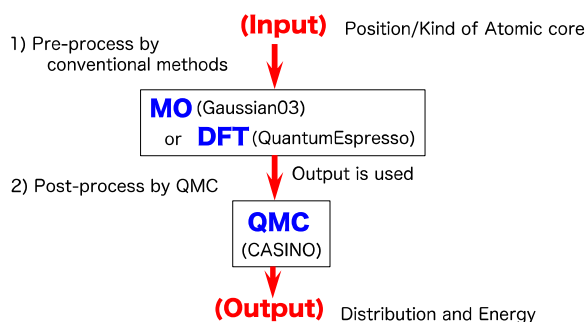
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### ABSTRACT

**Keywords:** QMC, DMC, Electronic correlation, Ab initio calculation

QMC (Quantum Monte Carlo method) electronic structure calculation is a first principles method based on the different strategy from that for conventional DFT (Density Functional Theory) or MO (Molecular Orbital) methods. In QMC, many-body WFs (Wave functions) are not decoupled into one-body functions and are subject to the projection operation which tunes a WF being closer to exact one, realizing the most reliable evaluation of electronic correlations beyond that by conventional methods. The method can be used as a post-processor to brush up the output obtained by the conventional DFT or MO methods. In the present talk, I'll show several published examples of such works. The discussions on the computational resources and international collaboration on this aspect are also given in the talk.



**Figure 1** .QMC ab initio calculation used for practical applications, a sort of a post-processing form.

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CHE-I-01

**Ryo Maezono** got his PhD (2000) in Applied Physics at Tokyo University. He was a JSPS fellow (Tokyo University/1999-2000). He got a postdoctoral position at Cavendish Laboratory, Cambridge University (2000-2002), and a tenure researcher at NIMS (National Institute of Materials Science, Japan (2001-2007). Now, he is a full Professor at JAIST (Japan Advanced Institute of Science and Technology), school of Information Science, working on Diffusion Monte Carlo (DMC) electronic structure calculations using massive parallel computations.

## CHE-I-02

# Diffusion Monte Carlo simulations applied to noncovalent systems

Kenta Hongo\*

*RCACI (Research Center for Advanced Computing Infrastructure), JAIST (Japan Advanced Institute of Science and Technology), Asahidai 1-1, Nomi, Ishikawa, 923-1292, Japan*

*\*E-mail: kenta\_hongo@mac.com; Tel. +81 761 51 1301*

### ABSTRACT

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**Keywords:** *Diffusion Monte Carlo, Noncovalent Systems, Molecular Interactions*

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Diffusion Monte Carlo (DMC) is known to be one of the most promising first-principles simulations to accurately reproduce electron correlation effects [1-2]. In the past two decades, its target systems have changed from atoms and molecules [3-5] to larger and more complicated systems [6-11]. This is because recent advances in high performance computing facilities provide massively parallel computing resources that match the essentially parallel algorithm in DMC. In this presentation, I will talk about DMC applications to noncovalent systems whose molecular interactions are difficult to be evaluated accurately by the other methods.

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**CHE-I-02**

**Kenta Hongo** received his Ph.D. from Tohoku University in 2005. After his postdoctoral at Tohoku University and Harvard University, he joined to JAIST in 2012 and was promoted to Associate Professor at Research Center for Advanced Computing Infrastructure (2017). He is now in charge of managing high-performance computing (HPC) facilities in JAIST. Using the HPC systems, he is working on materials simulations and informatics



# CHE-I-03

## Recent progress in the ab-initio quantum Monte Carlo code “TurboRVB”

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### ABSTRACT

**Keywords:** Quantum Monte Carlo, QMC, TurboRVB, Turbo-Genius

First-principles quantum Monte Carlo (QMC) techniques<sup>[1]</sup>, such as variational quantum Monte Carlo (VMC) and diffusion quantum Monte Carlo (DMC), are state-of-the-art numerical methods to obtain highly accurate many-body wave functions. These methods are useful when tackling challenging compounds that cannot be handled correctly within the DFT framework. I will talk about two recent improvements in our QMC code, TurboRVB<sup>[2,3]</sup>, in this presentation.

The first topic is dimer calculations. Calculations of the binding energies of dimers are the most fundamental benchmark of the ab-initio method. Nevertheless, it is still not easy to reach the so-called chemical accuracy ( $\sim 1$  kcal/mol) for several challenging molecules<sup>[4]</sup>, even by state-of-the-art numerical methods such as the diffusion Monte Carlo, due to several limitations. To overcome the difficulty, we have recently implemented the Pfaffian ansatz to our TurboRVB code. The Pfaffian is the most general implementation of the symmetric antisymmetrized geminal power (AGP) wavefunction<sup>[3,5]</sup>. The very flexible ansatz enables us to reach the chemical accuracy in the binding energy calculations even for challenging molecules such as C<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, and Na<sub>2</sub><sup>[6,7]</sup>.

The second topic is a workflow system for QMC calculations. We are currently developing a python wrapper for TurboRVB, called Turbo-Genius<sup>[3]</sup>, to “automatize” the complicated optimization procedure of a many-body wave function. The wrapper also makes it much easier to prepare input files, analyze output files, and perform advanced calculations. I will show fundamental features and several applications of the wrapper.

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CHE-I-03

**Kosuke Nakano** received his B.Sc. from Kyoto University in 2008, M.Sc. from Kyoto University in 2012, and Ph.D. from JAIST in 2017. Currently, he is an Asst. Prof in JAIST and a visiting researcher in SISSA. His research interests focus on quantum Monte Carlo, density functional theory, and materials informatics.

# CHE-I-04

## Superlarge-Scale Molecular Dynamics Simulations on Wear, Corrosion, and Cracking Mechanisms

Momoji Kubo<sup>1,\*</sup>

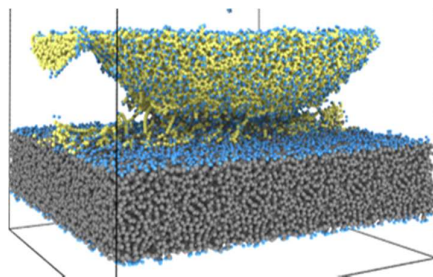
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### ABSTRACT

**Keywords:** *Reactive Molecular Dynamics, Chemical Reaction, Wear, Corrosion, Cracking*

Revealing wear, corrosion, and cracking mechanisms of materials is strongly required to realize safe and secure society. The theoretical guideline for the design of high-tolerance and high-durability materials should be established. Therefore, we developed a superlarge-scale reactive molecular dynamics simulation code “LASKYO” for clarifying chemical reaction-induced wear, corrosion, and cracking [1-3]. Fig. 1 shows one example of the wear process simulation of diamond-like carbon interfaces. Superlarge-scale simulations successfully reveal both the chemical and mechanical wear. Especially, we found that the chemical wear induced by the chemical reactions strongly affect the mechanical wear. Finally, we propose here that the control of nano-scale chemical reactions is very effective to reduce the macro-scale wear, corrosion, and cracking amount.



**Figure 1.** Superlarge-Scale Wear Process Simulation of Diamond-like Carbon Interfaces

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**CHE-I-04**

**Momoji Kubo** received his PhD degree from Tohoku University, Japan in 1999. Currently he is a Director and Professor in Center for Computational Materials Science, Institute for Materials Research, Tohoku University. His research interests focus on superlarge-scale simulations on multi-physics and multi-scale processes of tribology, battery, fuel cell, etc.

# CHE-I-05

## Effect of SnO<sub>2</sub> Support on Degradation of Pt Anode in Polymer Electrolyte Fuel Cell: First-Principles Study

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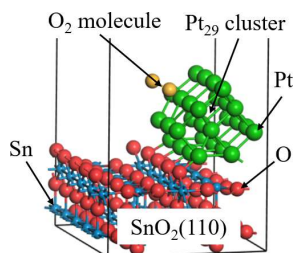
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### ABSTRACT

**Keywords:** First-principles Calculation, Polymer Electrolyte Fuel Cell, Degradation, Metal/Metal Oxide Composite

Polymer electrolyte fuel cell (PEFC) has advantages of small size and lightweight compared with other fuel cells. For the long operation of PEFC, it is necessary to suppress the degradation of anode materials in PEFC such as the poisoning of Pt catalyst by impurities (CO, NH<sub>3</sub>, and H<sub>2</sub>S) in fuel and dissolution of the polymer electrolyte membrane by OH radicals. Here, OH radicals are caused from H<sub>2</sub>O<sub>2</sub> generated by the chemical reaction of an O<sub>2</sub> molecule from the cathode with H<sub>2</sub> in fuel on the Pt catalyst. To increase the durability of PEFC, it is necessary to develop a Pt anode material, which can suppress the H<sub>2</sub>O<sub>2</sub> generation. In this study, we focused on a Pt/SnO<sub>2</sub> composite catalyst with high CO poisoning resistance, and H<sub>2</sub>O<sub>2</sub> formation on the Pt/SnO<sub>2</sub> composite catalyst was investigated by first-principles calculation.



**Figure 1** Models of Pt<sub>29</sub>/SnO<sub>2</sub>(110).

Firstly, by calculating O<sub>2</sub> adsorption energies, we investigated the adsorption process of an O<sub>2</sub> molecule, which is the initial step in the H<sub>2</sub>O<sub>2</sub> generation process. For the Pt/SnO<sub>2</sub> composite model, a Pt<sub>29</sub> cluster is put on SnO<sub>2</sub>(110) as shown in Fig. 1. The O<sub>2</sub> adsorption energy on the Pt<sub>29</sub> cluster of Pt<sub>29</sub>/SnO<sub>2</sub>(110) is 20.0 kcal/mol, while that on SnO<sub>2</sub>(110) is 3.60 kcal/mol. This indicates that the O<sub>2</sub> molecule preferentially adsorbs on the Pt catalyst of Pt<sub>29</sub>/SnO<sub>2</sub>(110) during H<sub>2</sub>O<sub>2</sub> generation. Usually, to increase electric conductivity, oxygen defects are introduced to SnO<sub>2</sub> support. To reveal the effect of the oxygen defect on the O<sub>2</sub> adsorption, we calculated the O<sub>2</sub> adsorption energy on the SnO<sub>2</sub>(110) surface with the oxygen defects [SnO<sub>2-x</sub>(110)]. The O<sub>2</sub> adsorption energy on the SnO<sub>2-x</sub>(110) is 41.8 kcal/mol, which is higher than that on the Pt catalyst on Pt<sub>29</sub>/SnO<sub>2</sub>(110) (20.0 kcal/mol). This indicates that O<sub>2</sub> molecule preferentially adsorbs on the SnO<sub>2</sub>(110) with the oxygen defect. Thus, we suggest that the oxygen defects induce the O<sub>2</sub> adsorption on the SnO<sub>2</sub> support and suppress the O<sub>2</sub> adsorption on the Pt catalyst of the Pt/SnO<sub>2</sub> composite.

### ACKNOWLEDGMENTS

This work was supported by funds from the New Energy and Industrial Technology Development Organization (NEDO) of Japan.

**CHE-I-05**

**Nobuki Ozawa** received his Ph.D. degree from Osaka University in 2009. Currently, he is an Associate Prof. at Tohoku University. His research interests focus on the degradation of anode catalysts and computational design of the high durability materials in polymer electrolyte fuel cell via density functional theory.

# CHE-I-06

## Molecular Dynamics Study on the Super-low Friction Mechanism of Silicon Carbide in Water

Yusuke Ootani<sup>1,\*</sup> and Momoji Kubo<sup>1</sup>

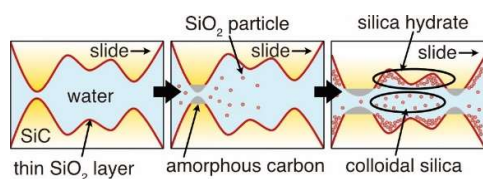
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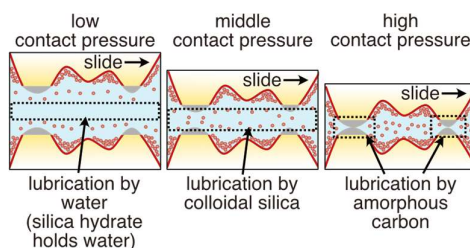
### ABSTRACT

**Keywords:** Molecular Dynamics, Tribology, Super-low Friction, Water Lubrication

Reduction of friction is crucial to reduce the energy loss of machine systems, thus various type of lubrication techniques are widely studied. Water is one of the promising clean lubricant<sup>1,2</sup>. Though water does not work as lubricant due to its low viscosity in general, it reduces the friction coefficient of silicon carbide (SiC) as small as 0.01 (so called super-low friction coefficient) due to the self-formation of a lubricant film by chemical reaction. However, the detailed mechanism is still in debate. Therefore, in this work, we performed molecular dynamics based sliding simulation to elucidate super-low friction mechanism of water. We found that water selectively oxidized the Si atoms, and thus Si atoms were removed from the surfaces as SiO<sub>2</sub> wear particles (Figure 1 center). The SiO<sub>2</sub> wear particles dissolved in water; colloidal silica layer was self-formed<sup>3</sup>. The part of SiO<sub>2</sub> wear particles deposited on the surfaces. The SiO<sub>2</sub> deposit contained water: silica hydrate layer was self-formed on the surface<sup>3</sup>. In contrast, the C atoms remains on the surfaces and forms an amorphous carbon layer on the surfaces (Figure 1 right). We proposed that the self-formed colloidal silica, silica hydrate, and amorphous carbon reduce friction in different contact pressure regime (Figure 2).



**Figure 1.** Schematic illustration of the lubricant layer formation process.



**Figure 2.** Schematic illustration of the sliding interface in different contact pressure regime.

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CHE-I-06

**Yusuke Ootani** received his PhD degree from Hokkaido University in 2011. Currently he is a Assistant Prof in Institute for Materials Research, Tohoku University. His research interests focus on mechanochemistry, tribology, and applications in molecular dynamics simulation.

## **CHE-I-07**

**Prof Emiel J.M. Hensen**

## CHE-I-08

# Hierarchical Multiscale Catalytic Modelling: From the active site to the reactor

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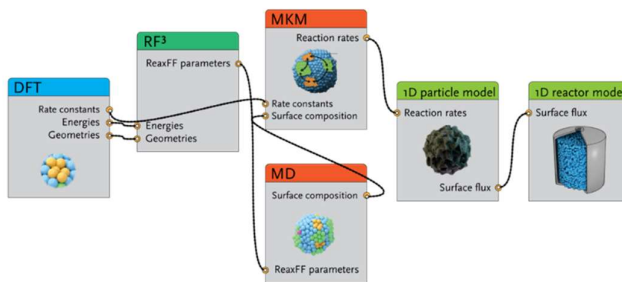
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### ABSTRACT

**Keywords:** Multiscale Modeling, DFT, Heterogeneous Catalysis, Fischer-Tropsch

Rational design of catalytic materials can be achieved using advanced methods that model the multiscale catalyst behaviour from the active site at the nanoscale to the reactor at the macroscale. Such methods are currently rather limited as they lack a proper description of the mesoscale. This leads to oversimplified models, wherein it is typically assumed that the catalytic activity is fully described by a single active site on a single surface facet. Catalytic nanoparticles are composed of many facets, each harbouring one or more active sites that have characteristic activity and selectivity patterns. These active sites are furthermore kinetically linked via diffusion processes over the catalyst nanoparticle and via adsorption/desorption processes with the surrounding gas phase. A proper description of catalytic nanoparticles thus encompasses all these phenomena, which occur on the mesoscale. As this scale is computationally inaccessible at the density functional theory level of theory, models are required that operate at the interplay of sufficient chemical accuracy and feasible computational costs.

In this talk, I will provide a step-by-step introduction how multiscale modelling in heterogeneous catalysis is achieved by using a combination of density functional theory, molecular dynamics, microkinetics modelling and reactor modelling.



**Figure 1.** Schematic depiction of multiscale modelling in heterogeneous catalysis.



CHE-I-08

**Ivo Filot** is an assistant professor at Eindhoven University of Technology. His research involves developing new computational techniques in multiscale modeling of catalytic reactions, in particular for the elucidation of the complex Fischer-Tropsch reaction mechanism, employing density functional theory and microkinetic modeling.



# CHE-I-09

## Steric vs Electronic Effects: A New Look into Stability of Diastereomers, Conformers and Constitutional Isomers

Sopant Datta and Taweetham Limpanuparb\*

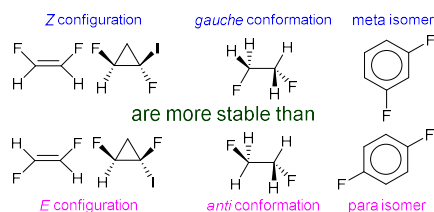
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### ABSTRACT

**Keywords:** Steric effect; electronic effect; cis effect; gauche effect

A quantum chemical investigation of the stability of compounds with identical formulas was carried out on 23 classes of halogenated compounds made of H, F, Cl, Br, I, C, N, P, O and S atoms. All possible structures were generated by combinatorial approach and studied by statistical methods. The prevalence of formula in which its Z configuration, gauche conformation and meta isomer are the most stable forms is calculated and discussed. Quantitative and qualitative models to explain the stability of the 23 classes of halogenated compounds were also proposed.



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CHE-I-09

**Taweetham Limpanuparb** is an Associate Professor of Theoretical Chemistry at Mahidol University. He is a recipient of the Young Scientist Award (2020), a prestigious award for young researcher in Thailand. He earned his PhD in Quantum Chemistry from the Australian National University (2012). His research interests include computational chemistry and science education.

# CHE-I-10

## Multiscale computational-experimental protocol for stability evaluation of catalysts in gas-phase reactions

**Supareak Prasertthdam<sup>1,\*</sup>, Meena Rittirum<sup>1</sup>, and Tinnakorn Saelee<sup>1</sup>**

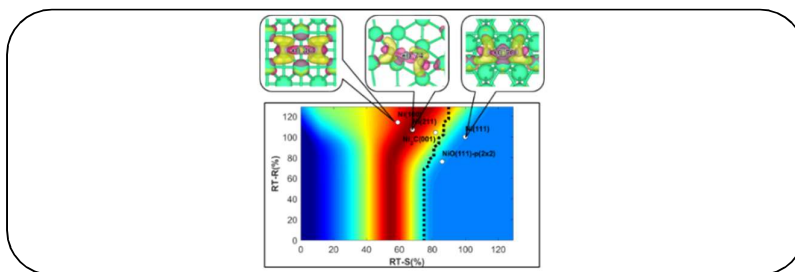
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### ABSTRACT

**Keywords:** Multiscale modeling, Density Functional Theory (DFT), Heterogeneous Catalysts, Chemical Reaction Engineering, Catalyst stability

The stability of catalysts is one of important factors apart from their activity. Hence, the evaluation protocol must be derived for the discovery of highly active and stable catalysts. As the computational-experimental materials screening is getting more attention due to the reduction of time and materials used along the process compared to the pure experimental screening, here, we present the multiscale computational-experimental protocol for the screening of active and stable catalysts, especially for the gas-phase reaction, in which the case of the methane reforming reaction was investigated. This protocol combining with the computational fluid dynamics simulation (CFD) that considers the profile of the reaction of interest in a reactor model. Hence, the catalyst screening from nano-scale up to the reactor-scale is introduced based on the case of the reforming catalysts.



**Figure 1.** Computational catalyst screening scheme via the Ratings concept

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**CHE-I-10**

**Dr. Supareak Prasertthdam** got his Ph.D. in Chemical Engineering from Texas A&M University (2018). He is the principal investigator of the CECC-HCU and the lecturer at the Department of Chemical Engineering, Chulalongkorn University. His research focuses on multi-scale materials modeling for catalytic materials screening combining first-principle methods, computational fluid dynamics, and chemical process simulations.

# CHE-I-11

## Active Site Dynamics and Mechanism of Arabinan Hydrolysis by Inverting GH43 Arabinanases: A QM/MM Study

Wijitra Meelua<sup>1,2</sup>, Tanchanok Wanjai<sup>1</sup>, Natechanok Thinkumrob<sup>2</sup>, Julianna Oláh<sup>3</sup>,  
Jon I. Mujika<sup>4</sup>, James R. Ketudat-Cairns<sup>5</sup>, Supa Hannongbua<sup>6</sup> and  
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### ABSTRACT

**Keywords:** Endo-1,5- $\alpha$ -L-Arabinanases, Enzyme Mechanism, Conformational Itinerary, QM/MM, SCC-DFTB

The endo-1,5- $\alpha$ -L-arabinanases, belonging to glycoside hydrolase family 43 (GH43), catalyse the hydrolysis of  $\alpha$ -1,5-arabinofuranosidic bonds in arabinose-containing polysaccharides. These enzymes are proposed targets for industrial and medical applications. Here, molecular dynamics (MD), potential energy surface and free energy (potential of mean force) simulations are undertaken using quantum mechanics/molecular mechanics (QM/MM) potentials to understand the active site dynamics, catalytic mechanism and the electrostatic influence of active site residues of the GH43 endo-arabinanase from *G. stearothermophilus*. The calculated results give support to the single-displacement mechanism proposed for the inverting GH43 enzymes: first a proton is transferred from the general acid E201 to the substrate, followed by a nucleophilic attack by water, activated by the general base D27, on the anomer carbon. A conformational change ( ${}^2E \leftrightarrow E_3 \leftrightarrow {}^4E$ ) in the  $-1$  sugar ring is observed involving a transition state featuring an oxocarbenium ion character. Residues D87, K106, H271 are highlighted as potential targets for future mutation experiments in order to increase the efficiency of the reaction.

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CHE-I-11

**Jitrayut Jitonnorn** received his PhD degree from Chiang Mai University in 2011. Currently he is an associate professor in theoretical chemistry at University of Phayao. His research interests focus on computational chemistry, enzyme catalysis and the applications in quantum mechanics/molecular mechanics (QM/MM) method and density functional theory (DFT).

# PFD-I-01

## Molecular Simulations of Bio-Interfaces for Sensor Development

Tiffany R. Walsh<sup>1</sup>

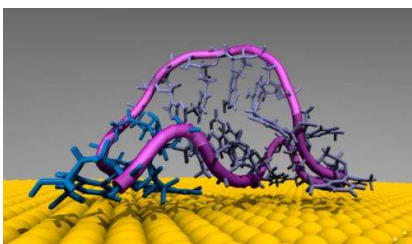
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### ABSTRACT

**Keywords:** *molecular simulations, graphene, gold, aptamers, biomolecules, sensors*

The interface between biomolecules and solid surfaces or nanoparticles is relevant to a range of defence areas including photonics and plasmonics, energy generation and harvesting, armour and protection, and biosensing.<sup>1</sup> To drive these applications forward, we need to understand how to manipulate the structures of these biomolecules adsorbed at the nano-interface. In partnership with experimental characterization, molecular simulations (Figure 1) can bring unique insights into these interfacial structures.<sup>2</sup> Our team specialise in the development and deployment of advanced molecular simulation techniques for these purposes. Here, I will summarize our collaborative developments with experimental researchers<sup>3</sup> to determine structure/property relationships of these interfaces.



**Figure 1.** Snapshot taken from a molecular dynamics simulation of a DNA hairpin adsorbed on the Au(111) surface (water not shown).

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**PFD-I-01**

**Tiffany Walsh** earned her PhD degree from University of Cambridge. She held a Glasstone Fellowship in Dept of Materials at the University of Oxford, and joined the Dept. of Chemistry, University of Warwick. She is a Professor of Bio/Nanotechnology at the Institute for Frontier Materials, Deakin University. Her research interests focus on computational modelling the interface between soft matter and synthetic materials.

## PFD-I-02

# Molecular Dynamics Simulations of the Self-Assembly of Drug-Delivery Vehicles

Chris Lorenz

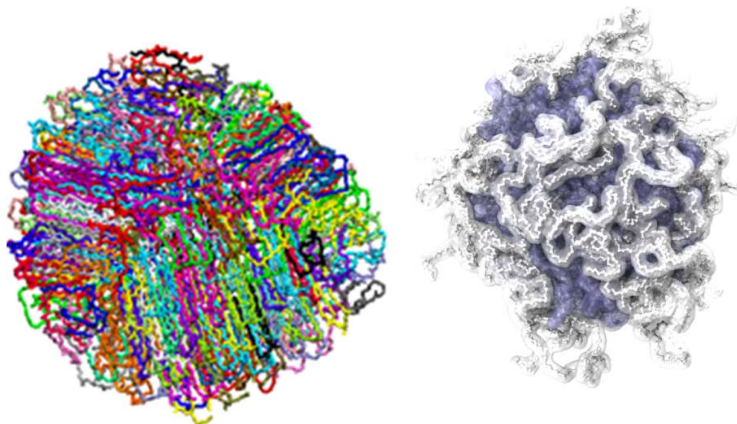
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### ABSTRACT

**Keywords:** *Molecular dynamics, polymers, lipids, drug-delivery, self-assembly*

Nanomedicine has continuously been in the spotlight according to the immense popularity of nanoscience and nanotechnology. Engineered nanomaterials have been specifically designed for various applications, including drug delivery, biomedical imaging, bio-sensing, diagnostics and therapy. Both polymer- and lipid-based nanoparticles have received intensive attention in the area of drug delivery systems because the hydrophobic drug molecules can be encapsulated in these self-assembled nanoparticles. In order to optimise the design of these drug-delivery vehicles, knowledge of the interactions that govern their self-assembly and the encapsulation of small molecules. Molecular dynamics simulations are frequently used as a tool to gain insight into the molecular scale interactions that govern the behaviour of materials of all types. In this talk, I will present the recent work done in my group in which we have used molecular dynamics simulations to investigate solid-lipid nanoparticles and polymeric nanoparticles. In both cases, I will demonstrate how we have used our simulations alongside complimentary experimental methods to provide as detailed a multi-scale picture of these systems as possible.



**PFD-I-02**

**Chris Lorenz** got his PhD in Chemical Engineering from the University of Michigan (2001). Currently he is a Professor in Physics in the Biological Physics and Soft Matter Group in the Department of Physics, King's College London. His research interests focus on the application of molecular dynamics simulations to investigations of a variety of problems in the areas of soft-matter self-assembly and biophysics.



## PFD-I-03

# Molecular Simulations from Physicists' Point of View: Applications for Biosensors, Polymers, and Proteins

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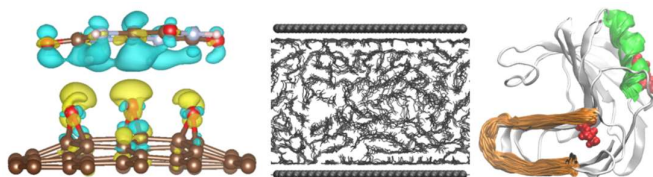
### ABSTRACT

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**Keywords:** *Molecular Simulations, Biosensors, Protein Engineering*

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This talk presents basic principles of molecular simulation techniques and some previous examples of visualizing molecular systems in atomistic details that help solving some challenge problems in biosensing, polymers, and protein engineering. Firstly, fundamental of electrochemical selectivity enhancement for ascorbic acid (AA), dopamine (DA), and uric acid (UA) was unveiled both by density functional theory (DFT) calculations and atomistic molecular dynamics (MD) simulations [1]. The simultaneous detection of the AA/DA/UA system has been an open problems in the field of biosensing. Then, another problem on the local glass transition of polymers induced by carbon-based fillers was investigated. A microscopic point of view on the molecular motion led to the total understanding of local transition from the 'rubbery' into the 'glassy' regime and the connection between microscopic and the macroscopic worlds [2]. Finally, two applications on protein engineering are mentioned: (1) two single-point mutations led to a synergistic effect that enhance the protein stability [3] and (2) the mechanisms of how protonation of lysozymes at low pH induced the formation of beta structures was also clarified [4].



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**PFD-I-03**

**Thana Sutthibutpong** received his PhD degree from the University of Leeds in 2015. Currently he is a Asst Prof in the Department of Physics, KMUTT. His research interests focus on applying molecular simulation techniques to explain molecular mechanisms underlying biomolecules and materials..

# BIO-I-01

## Structure based drug design of histone deacetylase inhibitors: lessons learned from computational studies and X-ray crystallography

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### ABSTRACT

**Keywords:** Epigenetics, Drug Design, Histone Deacetylases, Docking, Molecular Dynamics

Histone deacetylases (HDACs) are important modulators of epigenetic gene regulation and additionally control the activity of non-histone protein substrates. While for HDACs 1-3 and 6 many potent selective inhibitors have been obtained, for other subtypes much less is known on selective inhibitors and the consequences of their inhibition. In the present talk the structure based design of isoform selective HDAC inhibitors will be discussed. Docking studies using available crystal structures have been used for structure-based optimization of several series of compounds. We have investigated the role of HDAC6, HDAC8 and HDAC10 in the proliferation of cancer cells and optimized hits for potency and selectivity, both in vitro and in cell culture.1-3 The combination of structure-based design, synthesis, in vitro screening to cellular testing resulted in potent and selective HDAC8 inhibitors that showed anti-neuroblastoma activity in cellular testing.1,2 A second project focused on the development of isoform specific inhibitors of parasitic HDACs. Structure based design and crystallization resulted in the development of *Schistosoma mansoni* HDAC8 inhibitors for the treatment of bilharzia.4-6 In the present talk results from the computational studies including large ligand docking and molecular dynamic simulations are presented and discussed in the context of the obtained crystal structures of HDAC-inhibitor complexes.

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BIO-I-01

**Wolfgang Sippl** got a PhD in Pharmaceutical Chemistry at the University of Duesseldorf and was a post-doctoral fellow at the Universite Louis-Pasteur in Strasbourg (France). He was a full professor for Medicinal Chemistry, University of Halle-Wittenberg in 2003. Since 2010, he is a director of the Institute of Pharmacy in Halle. His main interests are computational chemistry and structure-based drug design.

## BIO-I-02

### Theoretical analyses on membrane permeability

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#### ABSTRACT

**Keywords:** Molecular Dynamics Simulations, Drug Design, Membrane Permeability, LogP

In recent years, middle-sized molecular drugs have attracted much attention from both industrial and pharmaceutical views in drug discovery because they possess advantages of both small drugs and antibodies. However, the physical properties of cyclic peptides have not been sufficiently understood. For example, there is no evaluation list on membrane permeability, and thus ADME has not been established. Therefore, it is worth investigating the membrane permeability of these molecules by theoretical methods. One of the alternative physical quantities for estimating the membrane permeability is a partition coefficient between octanol and water,  $\log P_{o/w}$ , which is calculated by the following equation.

$$\log P_{o/w} = \frac{\Delta G_{\text{wat}} - \Delta G_{\text{oct}}}{2.301RT}$$

where  $\Delta G_{\text{wat}}$  is the solvation free energy for water,  $\Delta G_{\text{oct}}$  is that for n-octanol,  $R$  is the gas constant, and  $T$  is the absolute temperature. Approximately 200 compounds, mainly low- to medium-molecular-weight organic compounds, were calculated using the *ab initio* and semiempirical methods with the self-consistent reaction field (SCRF) method with Gaussian16 [1]. Using the PM7/SMD and multi-regression method, we have achieved a good correlation between experimental and calculated  $\log P_{o/w}$  values [2].

Also, we have performed target molecular dynamics (tMD) simulations during membrane permeation processes using NAMD [3]. The target molecule used here is the syringolin A (SylA) and derivatives, which have a 12-membered cyclic peptide and exhibit weak proteasome inhibitory activity. In these simulations, the artificial force was applied to the center-of-mass of the chain. For each molecule, three trials were conducted from different initial conditions. The probability of membrane permeation was measured by changing the magnitude of the force in the range from 1 nN to 2 nN in tMD. We qualitatively confirmed the differences in permeation behaviors of three SylA derivatives, which is consistent with the experimental results.

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BIO-I-02

**Yasuteru Shigeta**, a Theoretical Chemist and Biophysicist, graduated from Department of Chemistry, Osaka University and obtained a Doctor of Science degree at there in 2000. He joined University of Tsukuba as a full professor since 2014. He has published more than 240 scientific papers and received several awards, especially, Ministry of Education, Culture, Sports, Science, and Technology (MEXT) Japan in 2010.



## BIO-I-03

# Second Coordination Effects in Blue Copper Protein with Combined Experimental and Computational Chemistry

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### ABSTRACT

**Keywords:** Noncovalent weak interactions, X-ray crystallography, XAS, DFT, QM/MM

Noncovalent weak interactions (< 10 kJ/mol) originated from the dispersion force have been recognized as important factor in many biological systems[1]. The effects of second coordination sphere on the tuning of active site were studied in a blue copper protein, pseudoazurin (PAz). The electrospray mass spectrometry and circular dichroism spectroscopy showed the stability of Met16 variants differ significantly due to the noncovalent weak interaction in second coordination sphere (Figure 1)[2,3]. The S and Cu K-edge XAS aided by computational simulations of Met16 variants showed that the Cu-S(Cys78) covalency is well correlated with the spectroscopies of type 1 copper site[4]. The high-resolution crystal structure analyses identified S- $\pi$ /CH- $\pi$  interaction in wild type PAz, face-to-face/face-to-edge  $\pi$ - $\pi$  interaction in Met16Phe variant, double CH- $\pi$  interaction in Met16Leu, and single CH- $\pi$  interaction in Met16Val and Met16Ile variants in the second coordination sphere. The computational chemistry simulations clarified these interactions with QM/MM (ONIOM) models. The energetic difference of noncovalent weak interaction clarified the structural stability, electronic structure and spectroscopic properties of PAz through the S- $\pi$ ,  $\pi$ - $\pi$ , CH- $\pi$  noncovalent weak interactions.

PAz	Met16Ile	Met16Val	WT	Met16Leu	Met16Phe
16th amino acid (2nd coordination sphere)					
His81 (Coordination sphere)					
Abundance of Folded-holo form	7 % (pH 3.5)	44 % (pH 3.5)	74 % (pH 3.4)	80 % (pH 3.4)	93 % (pH 3.4)
Relative Stability	Less Stable			More Stable	

**Figure 1.** The noncovalent weak interactions in the second coordination sphere in function with the structural stability (abundance of folded-holo form in pH 3.4-3.5)

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BIO-I-03

**Takahide Yamaguchi** received his PhD degree from Ibaraki University in 2016. Currently he is an Asst Prof in Ibaraki University. His research interests focus on metalloproteins

# BIO-I-04

## Computational prediction and interpretation of anticancer activities of peptides using a flexible scoring card method

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### ABSTRACT

**Keywords:** anticancer peptide; peptide; flexible scoring card method; propensity score; machine learning.

In this study, we develop and propose a flexible scoring card method (FSCM) with estimating propensity scores of local and global sequential information for the development of a sequence-based anticancer peptide (ACP) predictor (named iACP-FSCM) in order to improve the prediction performance and model interpretability [1]. Specifically, the FSCM method is employed to further improve the prediction accuracy and interpretability by utilizing both local and global sequential information of peptides. Both cross-validation and independent tests results revealed that the local sequential information played a crucial role in distinguishing ACPs from non-ACPs than that of the global sequential information. By comparing the iACP-FSCM and the state-of-the-art ACP predictors, we demonstrated that iACP-FSCM was the most suitable choice for ACP identification and characterization considering its simplicity, interpretability and generalizability. It is highly anticipated that the iACP-FSCM may be a useful tool for the rapid screening and identification of promising ACPs for clinical use. Due to the high potential of the FSCM method developed herein, this method could be easily applied for predicting and characterizing other antimicrobial peptides without any major modifications, such as antiviral peptides [2, 3] and antihypertensive peptides [2, 3], hemolytic peptides [4].

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**BIO-I-04**

**Watshara Shoombuatong** is an assistant professor in Center of Data Mining and Biomedical Informatics, Mahidol University. He has a specialty in QSAR modelling, machine learning, data mining, bioinformatics and computational biology, and protein and peptide sequence analysis. He is motivated to design and develop cutting-edge computational algorithms, models and pipelines in drug discovery and development.

## BIO-I-05

### Multiscale Simulations for Covalent Drug Design

**Alessio Lodola,<sup>1,\*</sup> Laura Scalvini,<sup>1</sup> Gian Marco Elisi,<sup>1</sup> Francesca Galvani,<sup>1</sup> Silvia Rivara,<sup>1</sup> and Marco Mor<sup>1</sup>**

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#### ABSTRACT

**Keywords:** Multiscale simulations, QM/MM, Drug Design

Quantum mechanical/molecular mechanical (QM/MM) multiscale approach is a well-established computational methodology for investigating biochemical reactions occurring in enzymes. From a drug discovery perspective, a detailed understanding of enzyme catalysis is fundamental to assist the design of covalent inhibitors targeting enzyme residues essential for the catalytic functioning.<sup>1</sup>

In the present talk, we summarize our experience in the field of QM/MM simulations applied to drug design problems which involved the optimization of compounds inhibiting well-known drug targets, including fatty acid amide hydrolase (FAAH), monoglyceride lipase (MGL), and epidermal growth factor receptor (EGFR). In this context, QM/MM simulations gave valuable information in terms of geometry (i.e., of transition states and metastable intermediates) and reaction energetics that allowed to correctly predict inhibitor binding orientation<sup>2</sup> and substituent effect on enzyme inhibition.<sup>3</sup> What is more, enzyme reaction modelling with QM/MM provided insights that were translated into the synthesis of new covalent inhibitors featured by a unique combination of intrinsic reactivity, on-target activity, and selectivity.

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**BIO-I-05**

**Alessio Lodola** received his PhD from the University of Pavia, in 2005. After a stint at the University of Bristol (UK), Dr. Lodola returned to Italy where he is now Associate Professor of Medicinal Chemistry at the University of Parma. Dr. Lodola's research focuses on the use of multiscale simulations for the design of endocannabinoid modulators, EGFR covalent inhibitors, and Eph-ephrin antagonists.

# CSE-I-01

## Neural Network Quantum Molecular Dynamics (NNQMD) for Water and Covalent Glasses

**Ken-ichi Nomura<sup>1</sup>, Nitish Baradwaj<sup>1</sup>, Shogo Fukushima<sup>2</sup>, Rajiv K. Kalia<sup>1</sup>, Aravind Krishnamoorthy<sup>1</sup>, Ankit Mishra<sup>1</sup>, Aiichiro Nakano<sup>1</sup>, Pankaj Rajak<sup>3</sup>, Kohei Shimamura<sup>2</sup>, Fuyuki Shimojo<sup>2</sup>, Priya Vashishta<sup>3</sup>**

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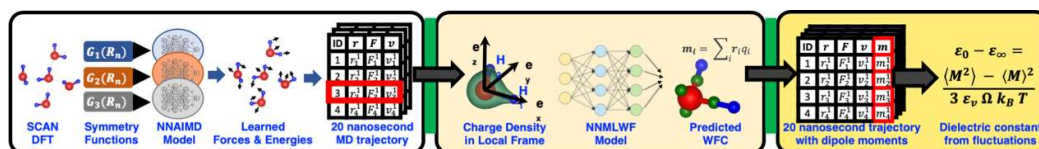
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### ABSTRACT

**Keywords:** Neural Network Molecular Dynamics, Machine Learning, Dielectric Constant, Intermediate-Range Order

Machine learning has become powerful tool in modern computational materials science. Among diverse applications, molecular dynamics (MD) simulation based on neural network (NN) has been attracting great attentions. With the highly accurate energy landscape encoded by ab-initio molecular dynamics training dataset, our goal is to develop an efficient and robust neural network quantum molecular dynamics (NNQMD) framework to perform multimillion atom and long-time nano seconds to microsecond simulations that provide unprecedented access to materials processes and properties. We have developed a scalable NNQMD simulation framework that has been successfully applied to different class of materials to compute their structural, dynamical and dielectric properties. In this talk, I will discuss our recent progress and applications to water and medium range order in covalent glasses systems.



**Figure 1.** NNQMD framework for dielectric constant calculation of water.

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**CSE-I-01**

**Ken-ichi Nomura** received his PhD degree from University of Southern California (USC) in 2008. Currently he is a Senior Lecturer in Materials Science at USC. His research interests focus on materials modelling using high-performance computing and machine learning.

## CSE-I-02

# Utilizing System and Hardware to Accelerate HPC

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### ABSTRACT

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**Keywords:** *Virtual Memory, GPU Design, Processing-in-memory, Accelerators Design*

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The increase in compute density on both the traditional CPU architecture as well as the high-throughput GPU architecture has enabled significant performance improvement across various types of modern applications including machine learning, AI, big data and bioinformatics. However, these applications' increasing resource demand also creates new challenges and opportunities for system and hardware designs. Rather than relying on software techniques to mitigate these new performance bottlenecks, this talk introduces novel hardware-software co-designs that can improve applications' performance across various domains through microarchitectural modification to modern hardware such as the high-throughput GPU, a traditional CPU with hybrid memory, or an application-specific accelerator. Specifically, this talk will provide two different case studies of these hardware changes. First, we will discuss architectural modifications to supercomputer and cloud infrastructure to enable even higher throughput to modern applications. Second, we will discuss how near-data processing and near-data accelerators can significantly reduce data transfer, leading to significant improvement in performance and energy efficiency.

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**CSE-I-02**

**Rachata Ausavarungnirun** received Ph.D. in Electrical and Computer Engineering from Carnegie Mellon University in 2017. Now he is an assistant professor at the Sirindhorn International Thai-German Graduate School of Engineering (TGGS) at King Mongkut's University of Technology North Bangkok. His research spans multiple topics across computer architecture and system software with emphasis on GPU architecture.



## CSE-I-03

# An Application of High-Performance Computing in Chemical Transport Model

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### ABSTRACT

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**Keywords:** Centre for Air Pollution Mitigation (CAPM), Weather Research Forecast Model (WRF), WRF-chem

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In 2020, National Environment Board approved to establish Center for Air Pollution Mitigation (CAPM) in order to support national agenda of haze situation which is driven by Ministry of Natural Resources and Environment and the alliances. Regarding to the component and responsibility of CAPM, Director General of Pollution Control Department is in charge as the director of CAPM and major tasks of CAPM are haze/air quality situation report for the whole country with meteorological conditions, knowledge transfer of haze/air pollution phenomena including significant sources of problem (e.g. open burning and transboundary haze) and “prediction of haze situation for 3 days in advance” in order to support preparation of daily life such as episode control for open burning and transportation. The chemical transport model (WRF-chem) developed by NOAA/USA was chosen as a major tool for haze prediction because the chemical mechanism inside WRF-chem can cope with both primary and secondary air pollutant. However, this kind of mathematical modelling requires vast processing resources which means an ordinary processing unit can not be used to perform this tool. Therefore, Pollution Control Department and National Electronics and Computer Technology Center (NECTEC) joined a collaboration of performing WRF-chem on high performance computing unit (TARA) since December 2020. The major simulation products represent critical areas such as Bangkok and Metropolitans and the northern part of Thailand with high resolution grid (3 km). For the future works, the preparation of whole country forecasting with more resolution and accuracy has been in progress.



**CSE-I-03**

**Sakda Tridech** received his PhD degree from Brunel University in 2012. Currently he is an Environmentalist and Director of Air Quality Model and Geographic Information Centre in Pollution Control Department, Ministry of Natural Resources and Environment.

# MST-I-01

## Mathematical modelling and its application

Usa Humphries

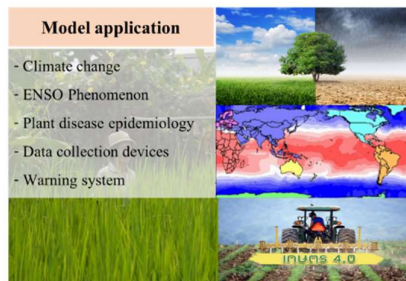
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### ABSTRACT

**Keywords:** Mathematical model, Plant disease, Climate change

Mathematical ideas can be used to describe the events or phenomena that occur in the real world. Mathematical modelling is just the translation of the behaviours into the language of mathematics. The models will allow us to simulate the behaviours when the value of the parameters in the model are changed when the environment change. It may help to explain a system and to study the effects of different components, and to make predictions about behaviour. Many plant diseases can be described by mathematical models including rice blast disease that is one of the most important diseases and outbreaks in the rice-growing areas around the world. The model can simulate the risk of rice blast disease under the climate changing conditions. Specific modelling methods such as model of rice blast disease under tropical climate conditions, model of plant pathogen epidemics with lesions growth and spatial dynamic and ENSO simulation are described, with an outline of their modelling and result. Current approaches for evaluation within plant disease and effects of the ENSO phenomenon on precipitation in Thailand are also briefly discussed.



**Figure 1.** Applications of mathematical models

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**MST-I-01**

**Usa Humphries** received Ph.D. degree in Applied Mathematics-University of Exeter, England. She is Associate Professor in Applied Mathematics, Department of Mathematics, King Mongkut's University of Technology Thonburi (KMUTT). Her research interests include numerical oceanic and atmospheric modeling, numerical method, weather and climate change, and data assimilation and data analysis.

## MST-I-02

# Computational mathematics: from new pseudoprimality notions to unravelling the structure of criminal networks

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### ABSTRACT

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**Keywords:** *Pseudoprimality, Generalised Lucas/Pell-Lucas sequences, Numerical simulations, social network analysis, resilient criminal networks, Sicilian Mafia.*

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Numerical simulations play a central role in the study of many practical problems.

The first focus of this talk is on numerical simulations and computational techniques used for studying new pseudoprimality concepts. Pseudoprimes are composite integers sharing properties of the prime numbers, with applications in areas including public-key cryptography. Here we present some novel classes of pseudoprimes related to generalized Lucas sequences, which recover many classical pseudoprimes as particular cases. We discuss computational tools which facilitated this work, associated integer sequences added to the Online Encyclopedia of Integer Sequences, then identify key properties, and formulate some conjectures.

A second focus of this talk is the simulation of criminal organisations using network science analysis. Using real data from criminal investigations, an international collaboration has investigated the structure and operations of two Sicilian Mafia families. Current studies involve the modelling and simulation of the dynamic behaviour of resilient criminal networks.

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**MST-I-02**

**Ovidiu Bagdasar** holds a PhD degree in Applied Mathematics from University of Nottingham in 2011, and a PhD in Pure Mathematics from UBB Cluj Romania, in 2015. Currently he is an Assoc Prof at the University of Derby, UK. His research interests include number theory, discrete mathematics, optimisation, simulations, applications of mathematics in data science.



# MST-I-03

## Cell Voltage Static-Dynamic Mathematical Modelling of a Proton Exchange Membrane Electrolyzer

Damien Guilbert<sup>1,\*</sup>

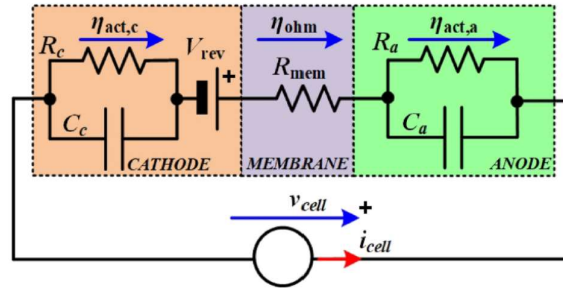
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### ABSTRACT

**Keywords:** PEM electrolyzer, Mathematical Modelling, Static-Dynamic, Adaptive Parameters

This presentation is focused on the proposal and experimental validation of a static-dynamic electrical model of a proton exchange membrane (PEM) electrolyzer. The originality of this work concerns the cell voltage modelling according to static and dynamic operations. Indeed, the cells of the PEM electrolyzer may be subjected to degradations due to the operating conditions and current ripple generated by power electronics. Hence, cell voltage response and efficiency may be affected. For this reason, it is crucial to model each cell voltage to investigate the degradation and wear effects mainly caused by the dynamic operating conditions met when coupling with renewable energy sources and current ripple from power electronics. To develop an accurate model, static and dynamic operations are investigated on a commercial-400 W PEM electrolyzer stack. To enhance the accuracy of the model in replicating the real behavior of the electrolyzer, the parameters of the model are adapted according to the input current. The comparison between the experimental data and the developed model has enabled confirming the effectiveness of the model to reproduce the cell voltage static and dynamic behavior according to the input current.



**Figure 1.** Equivalent electrical circuit of a cell of a PEM electrolyzer.



MST-I-03

**Damien GUILBERT** received Ph.D. degree in electrical engineering from University of Technology of Belfort-Montbéliard (UTBM) in 2014. He is Associate Professor at University of Lorraine and a permanent member of GREEN (Group of Research in Electrical Engineering of Nancy) laboratory. His research interests include power electronics for electrolyzer applications and proton exchange membrane electrolyzer modelling.

## ORAL PRESENTATION

# CHE-O-01

## Lithium Adsorption on Silicon Quantum Dots: A DFT Study

**Fadjar Mulya<sup>1</sup>, Thanawit Kuamit<sup>1</sup>, and Vudhichai Parasuk<sup>1,\*</sup>**

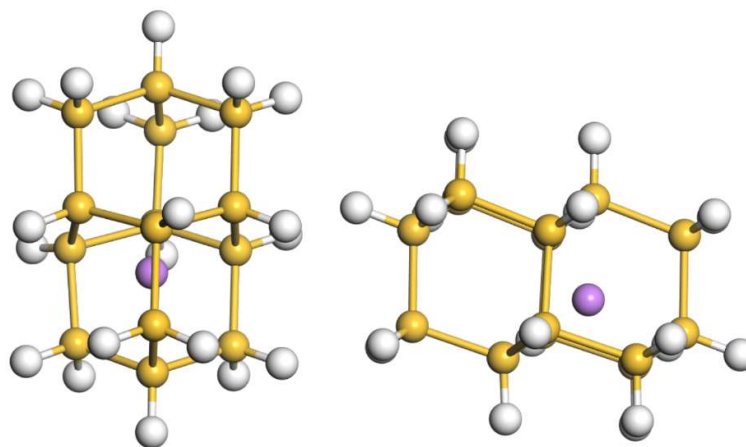
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### ABSTRACT

**Keywords:** DFT, Lithium-ion battery, Adsorption, SiQDS

Structural and electronic of hydrogenated silicon quantum dots (SiQDs) were studied using the density functional theory (DFT) method with M06-2X hybrid functional and 6-31G+(d) basis set using Gaussian09 software program. Effects of cluster size, adsorption sites of SiQDs (hollow, bridge and on-top), binding energy, bandgap energy, charge distribution, and adsorption behaviour are in good agreement with previous theoretical and experimental studies. The most stable structure which adsorbed lithium on SiQDs is in hollow adsorption site with binding energy 1.00 eV. The bandgap energy of SiQDs is in the range of 1.86 and 4.18 eV. This study recommends SiQDs for an anode material of high-energy-density lithium-ion rechargeable batteries.



**Figure 1.** Adsorption of Lithium on SiQDS

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## CHE-O-02

# Bimetallic Zr/Ti metal-organic framework for desulfurization at mild conditions

**Phakawan Thinsoongnoen<sup>1</sup>, Vetiga Somjit<sup>1</sup>, Taweesak Pila<sup>1</sup>, Pemikar Srifa<sup>1</sup>, and Kanokwan Kongpatpanich<sup>1,\*</sup>**

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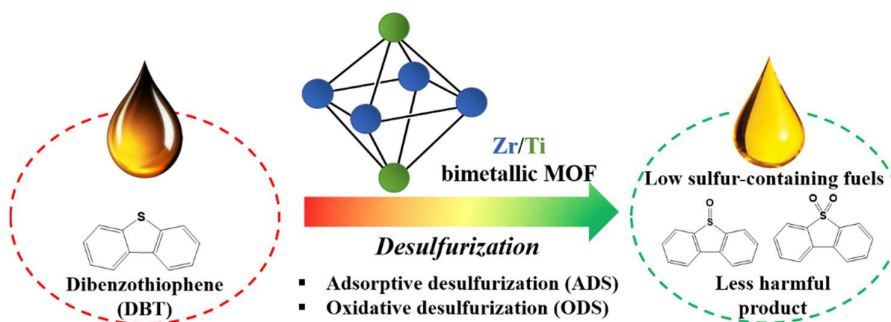
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### ABSTRACT

**Keywords:** Bimetallic metal-organic frameworks, Adsorptive desulfurization, Oxidative desulfurization, Density functional theory

Adsorptive desulfurization (ADS) and oxidative desulfurization (ODS) methods are two promising approaches to remove sulfur compounds from fuels owing to their milder operating conditions compared to hydrosulfurization. Metal-Organic frameworks (MOFs) are attractive porous materials that can be utilized as absorbents and heterogeneous catalyst for removal of Dibenzothiophene (DBT), which is the major sulfur-containing compound found in fuels. In this work, bimetallic Zr/Ti MOF has been developed to achieve a dual-function MOF for both ADS and ODS at mild conditions with high removal efficiency. The local structure of bimetallic metal center has been studied by combined X-ray absorption spectroscopy (XAS) and Density Functional Theory (DFT) calculation. The synergistic effect from the bimetallic metal center and the desulfurization mechanisms for both ADS and ODS will be demonstrated by product distribution analysis and DFT calculation.



**Figure 1.** Adsorptive desulfurization (ADS) and oxidative desulfurization (ODS) of DBT on Zr/Ti bimetallic MOF

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## CHE-O-03

# A DFT Study of Hydrodeoxygenation Reaction Mechanistic over MoP for Bio-Oil Treatment

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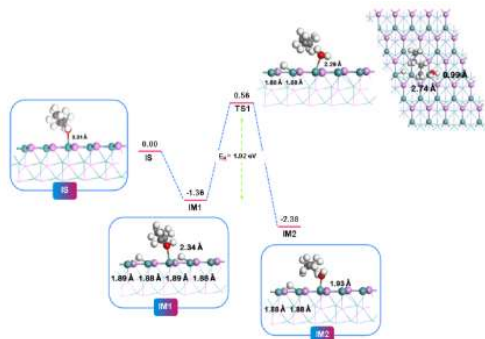
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### ABSTRACT

**Keywords:** hydrodeoxygenation (HDO); decarbonylation (DCO); density functional theory (DFT); transition metal phosphides (TMP); MoP catalysts

The transition metal phosphides (TMP) catalysts have been widely tested for hydrotreating applications, including deoxygenation (DX) of bio-oil surrogates. Molybdenum based catalysts such as Mo-terminated of MoP surface were reported to have high hydrodeoxygenation (HDO) conversion efficiency. In this work, we investigated the DX reaction mechanism of fatty acid to produce alkane on different planes (001 and 101) of Mo-termination of MoP surface using density functional theory (DFT) calculation. Here, important reaction pathways including hydrodeoxygenation (HDO) and decarbonylation (DCO) pathways, along with comprehensive elementary step reactions and rate limiting steps will be identified. The result showed that the deoxygenation reaction mechanisms is difficult via the HDO pathway and DCO pathway on (001) Mo-termination of MoP surface due to the large reaction barriers of 1.99 and 2.83 eV, respectively. Moreover, the deoxygenation reaction mechanism on (101) Mo-termination of MoP surface prefers HDO pathway rather than the DCO pathway; the energy barrier for the rate-limiting step is 1.92 eV. The insights received in this study will be substantially beneficial for the improvement of broad MoP catalysts for deoxygenation reaction mechanism.



**Figure 1** .The energy profile of the butanol conversion to butane pathway on )101(MoP

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# CHE-O-04

## Effect of External Electric Field on the Catalytic Performance of $\text{Fe}_3(\text{BTC})_2$ Metal-Organic Frameworks for CO Oxidation with $\text{N}_2\text{O}$ : A DFT Study

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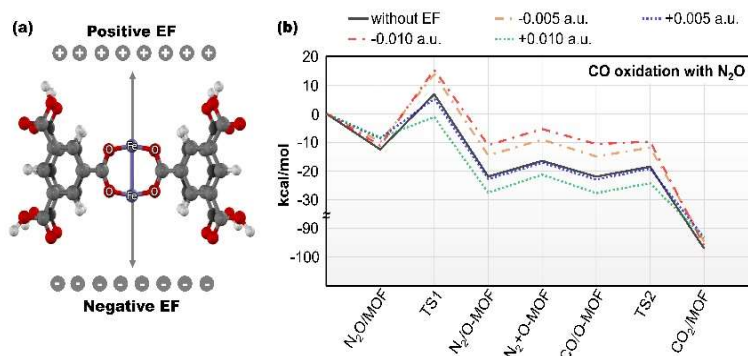
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### ABSTRACT

**Keywords:** CO Oxidation, Fe-BTC Metal-Organic Frameworks, External Electric Field, DFT

We investigate the effect of an external electric field (EF) on the oxidation of CO with  $\text{N}_2\text{O}$  over the metal-organic framework  $\text{Fe}_3(\text{BTC})_2$  (BTC=1,3,5-benzentricarboxylate) by means of density functional calculations using the M06-L functional. We apply the perpendicular EF to the  $\text{Fe}_3(\text{BTC})_2$  in the range of -0.010 to +0.010 a.u. The reaction is assumed to proceed in two steps, the N-O bond of  $\text{N}_2\text{O}$  breaking and the C-O bond formation. The calculated activation energies are 19.3 and 3.5 kcal/mol for the first and second steps without the EF. The applied EF is found to be an effect on all species along the reaction coordinate. The activation energies for the N-O bond breaking, the rate-determining step of the reaction, are reduced from 19.3 to 13.7 and 7.1 kcal/mol by applying positive EF of +0.005 and +0.010 a.u., respectively. In contrast, by applying negative EF, the barriers are increased to be 23.6 and 26.5 kcal/mol for -0.005 and -0.010 a.u., respectively. Based on charge transfer analysis, the applied positive EF can enhance the charge transfers from the catalytic site to the  $\text{N}_2\text{O}$  molecule antibonding leading to the higher activity for the N-O bond breaking. The results suggested that the applied external electric field can undoubtedly customize the catalytic activity of  $\text{Fe}_3(\text{BTC})_2$  for CO oxidation with  $\text{N}_2\text{O}$ .



**Figure 1.** The direction of EF applied in perpendicular direction to the  $\text{Fe}_3(\text{BTC})_2$  (a) and reaction energy profiles for CO oxidation with  $\text{N}_2\text{O}$  over  $\text{Fe}_3(\text{BTC})_2$  include the effect of applied EF (b).

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# CHE-O-05

## Multifactor Computational Screening of Materials for Renewable Energy Conversion and Storage

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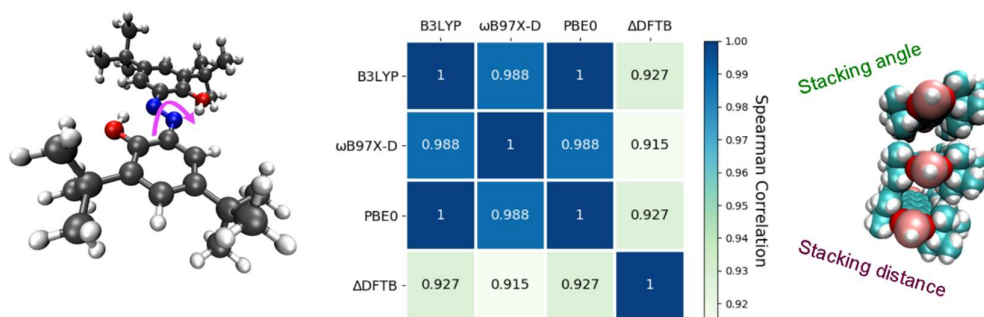
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### ABSTRACT

**Keywords:** covalent organic frameworks, solar thermal fuels, DFT, DFTB, machine learning

Nearly a decade after the Obama administration's launch of the Materials Genome Initiative in the US, the adoption of computational and data-driven approaches to materials discovery has accelerated across the global materials research community. These approaches require cooperation among domain experts in physical sciences and data science; junior scientists working in this field are developing domain knowledge in both areas simultaneously, becoming the first native "materials informaticians".<sup>1</sup>

In this talk, I will share some recent efforts of our team of budding materials informaticians to integrate a data-driven approach with our physics-based materials simulations of renewable energy materials. The overarching goal of these efforts is to enable high-throughput virtual screening of candidate materials for two specific applications: (1) photoactive covalent organic frameworks (COFs) for increasing solar energy conversion efficiency via singlet fission<sup>2</sup>; (2) photoisomerizable solar thermal fuels (STFs) for integrated solar energy conversion and storage<sup>3</sup>. From a physical sciences perspective, this talk will apply electronic structure models to elucidate strategies for optimizing two classes of photoactive materials for solar energy conversion and storage applications. From a data science perspective, this talk will highlight the challenges of data curation in the photoactive materials domain space and outline our strategy for addressing these challenges.



**Figure 1.** Correlating DFTB and DFT measurements of excited-state properties as a basis for predictive screening of organic materials for solar energy conversion

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## PFD-O-01

# A computational Fluid Dynamics (CFD) study on coke formation behavior over a spherical alumina-supported nickel catalyst (Ni/Al<sub>2</sub>O<sub>3</sub>) particle for dry reforming of methane

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## ABSTRACT

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**Keywords:** CFD, Dry reforming of methane, Coke formation

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Dry reforming of methane (DRM), the solid-catalyzed gas-phase reaction can convert greenhouse gases into synthetic gas. However, the coke formation over the catalyst particle is a major problem, which will lead to catalyst deactivation. In this work, the three-dimensional (3D) computational fluid dynamics (CFD) simulation with chemical reactions which was performed by commercial software ANSYS Fluent to investigate coke formation behaviour over a spherical alumina-supported nickel catalyst (Ni/Al<sub>2</sub>O<sub>3</sub>) particle. A single spherical catalyst particle model was used with a particle diameter of 2 mm and pore diameter of 10 nm. The CH<sub>4</sub>/CO<sub>2</sub> molar ratio of unity was used. The distribution of temperature, reactant and product profiles inside the catalyst particle were also analyzed. The results show good agreements with experimental data. In addition, the difference of coke accumulation between catalyst surface and within the particle zone was observed.

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## PFD-O-02

# Study of Heat and Mass Transfer in MHD Flow of Sutterby Nanofluid over a Curved Stretching Sheet with Magnetic dipole and effect

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### ABSTRACT

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**Keywords:** Chemical reactions, Curved surface, Heat transfer, Magnetic dipole, Thermal radiation, Sutterby ferrofluid

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A systematic study of non-Newtonian Sutterby ferrofluid and heat transfer in the flow due to curved stretching sheets is presented. Flow is caused by the linear velocity of the curved sheet. Concentration and energy equations are incorporated in the study of mass and heat transfer impacts. The motile microorganism equation included the swimming of the gyrotactic microorganism. The governing equations are transformed from partial differential equation to ordinary differential equation and the solved using Homotopy Analysis method. The velocity is reduced due to dipole and non-Newtonian parameters effects. Temperature increases with the dipole effect and thermal radiation parameters. Concentration decreases with an increase in the homogeneous chemical reaction parameter and the concentration of microorganisms decreases with the Lewis number. Streamlines show that trapping on the curved stretched surface is uniform.

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# PFD-O-03

## Biomechanical evaluation of screw configurations on conventional plate fixation in humeral shaft fracture using finite element analysis

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### ABSTRACT

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**Keywords:** *Humeral shaft fracture, Plate and screw fixation, Screw configurations, Finite element analysis*

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A standard technique of humeral shaft fracture treatment is plate and screw fixation . Bicortical screws are commonly used in this technique .However, previous studies reported that the tip of bicortical screws could damage radial nerve .To avoid the nerve injury, this study was evaluated the biomechanical properties and optimized the appropriate condition of screw configurations in the humeral shaft fracture using finite element analysis .Simple humerus models were allocated into six different screw length configurations .All models were tested in axial compression, torsion, and bending .The construct stability was investigated by stiffness, relative displacement, and von Mises stress .The non-inserted screw at the risk position of radial injury provided low stability which considered by the lowest stiffness in torsion, the highest relative displacement in torsion and bending, and the lowest von Mises stress compared to other configurations .At the risk position, there was no significant difference in bicortical, unicortical and unicortical abutting screw .These results suggested that the replacement of unicortical and unicortical abutting screw at the risk position could provide stability equivalent to bicortical screw fixation .Therefore, this finding may suggest the screw configurations to remove the risk of radial nerve injury .

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# PFD-O-04

## Biomechanical evaluation of four fixation methods in two-tunnel Coracoclavicular ligament reconstruction technique using Finite element analysis

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### ABSTRACT

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**Keywords:** AC joint dislocation, CC reconstruction, Evaluation of AC joint treatment, Finite element analysis

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To treat Acromioclavicular (AC) joint dislocation, the two-tunnel Coracoclavicular (CC) ligaments reconstruction technique is a recommended technique. However, there presents failures from this technique including tunnel widening and loss of reduction. Previous studies found that the multiple choice of fixation types may affect treatment failure. Therefore, this study aimed to investigate the stability and effect of four different fixation methods in two-tunnel CC ligament reconstruction technique using Finite element analysis (FEA). The simplified surgical procedures were created in four models, which different in tunnel positions and fixation methods. All models were applied 70 N load in three directions. Maximum von Mises stress and displacement were analysed. The maximum stress of clavicle bone in all models provided lower value than bone yield strength (114 MPa). Interestingly, perpendicular tunnel position with O-loop fixation generated lower stress value in all direction tests than other models. This fixation also exhibited the lowest displacement value in superior direction, which represented a good stability. Perpendicular tunnel position with O-loop fixation method may help to decrease risk of failure after treatment due to cumulative stress in the construct.

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# PFD-O-05

## ***In silico* study of signature interactions between methylated DNA and graphene oxide nanosheet for universal cancer screening**

**Unnop Srikulwong<sup>1</sup>, and Theerapong Paungmali <sup>1,\*</sup>**

<sup>1</sup>*Department of Physics, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand*

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### ABSTRACT

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**Keywords:** *Graphene oxide nanosheet; Methylated DNA; Molecular dynamics (MD) simulation; Density functional theory (DFT)*

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DNA methylation, an epigenetic process by which methyl groups are added to DNA, is associated with carcinogenesis. It could serve as a universal cancer biomarker [1]. Therefore, signature interactions between methylated DNA and nanomaterials such as graphene oxide (GO) can pave the way for DNA methylation detection. To unveil their macro- and micro-level mechanisms, molecular dynamics (MD) simulation and density functional theory (DFT) have been conducted. According to the MD simulations, methylated and unmethylated DNAs were adsorbed onto GO with different contacting surface areas (CSAs). The CSA of the methylated and unmethylated ssDNA in water were  $\sim 13 \text{ nm}^2$  and  $\sim 5 \text{ nm}^2$ , respectively, indicating that GO was more favourable for adsorption of methylated DNA. In the presence of divalent ions ( $\text{Mg}^{2+}$ ), the CSA of both cases was  $\sim 8 \text{ nm}^2$ , suggesting that different adsorption can be observed in water. Based upon DFT calculation, energy gap of pristine graphene (pG) and GO in the presence of 5-methylcytosine (5mC) were 1.6 and 12.9 meV, respectively, while the adsorption of cytosine resulted in lower energy gap (1.2 meV for pG and 9.5 meV for GO). The results in different electrical conductivity of GO will open the door for universal cancer screening approaches based on GO.

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## PFD-O-06

# A molecular dynamics study on the diffusion and imprint ability of spectinomycin under different sizes of aniline oligomers

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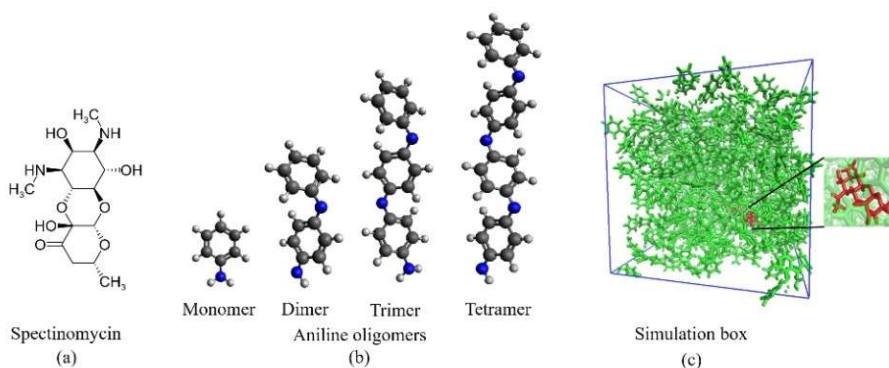
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### ABSTRACT

**Keywords:** Molecular dynamics simulation, Molecularly imprinted polymer, Aniline, Spectinomycin

Molecularly imprinted polymer (MIP) is the polymer created by molecular imprinting techniques that leaves cavity for the specific interactions with a template molecule, and has been applied in molecular selectivity tasks. In this study, molecular dynamics (MD) simulation was used to prove that aniline oligomer could be developed as an MIP for the detection and separation of the spectinomycin drug molecule for gonorrhoea treatment. MD simulations were performed to compare the mean square displacement (MSD) and the diffusivity of spectinomycin within aniline oligomers of different sizes. The calculations showed that the diffusion coefficient was significantly dropped when the size of aniline oligomer is more than two monomers. Then, the distances between pairs of aniline monomers were measured to monitor the geometry of cavity created when the spectinomycin is absent. The analysis showed that aniline tetramer sustained most of its cavity geometry and therefore the optimal oligomer size for further development of MIP.



**Figure 1.** Chemical structures and simulation setup for proved by MD; (a) spectinomycin that is template molecule; (b) aniline oligomer; and (c) 64 nm<sup>3</sup> simulation box that was added spectinomycin and anilines

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## PFD-O-07

# An exact analysis of unsteady MHD free convection flow of some nanofluids accounting heat radiation and injection/consumption

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## ABSTRACT

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**Keywords:** MHD, Laplace transform, Porous material, Nanofluid

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This article investigates the influence of ramped wall velocity and ramped wall temperature on time dependent, magnetohydrodynamic (MHD) natural convection flow of some nanofluids close to an infinitely long vertical plate nested in porous medium. Combination of water as base fluid and three types of nanoparticles named as copper, titanium dioxide and aluminum oxide is taken into account. Impacts of nonlinear thermal radiation flux and heat injection/consumption are also evaluated. The solutions of principal equations of mass and heat transfer are computed in close form by applying Laplace transform. The physical features of connected parameters are discussed and elucidated with the assistance of graphs. The expressions for Nusselt number and skin friction are also calculated and control of pertinent parameters on both phenomena is presented in tables.

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# PFD-O-08

## Unsteady Radiative Natural Convective MHD Nanofluid Flow Past a Porous Moving Vertical Plate with Heat Source/Sink

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### ABSTRACT

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**Keywords:** MHD, Volume fraction, Thermal radiation, Nanofluid

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In this research article, we investigated a comprehensive analysis of time-dependent free convection electrically and thermally conducted water-based nanofluid flow containing Copper and Titanium dioxide (Cu and TiO<sub>2</sub>) past a moving porous vertical plate. A uniform transverse magnetic field is imposed perpendicular to the flow direction. Thermal radiation and heat sink terms are included in the energy equation. The governing equations of this flow consist of partial differential equations along with some initial and boundary conditions. The solution method of these flow interpreting equations comprised of two parts. Firstly, principal equations of flow are symmetrically transformed to a set of nonlinear coupled dimensionless partial differential equations using convenient dimensionless parameters. Secondly, the Laplace transformation technique is applied to those non-dimensional equations to get the close form exact solutions. The control of momentum and heat profile with respect to different associated parameters is analyzed thoroughly with the help of graphs.

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# PFD-O-09

## Grid Spacing for Efficient Data Center CFD Simulation: A Preliminary Study

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### ABSTRACT

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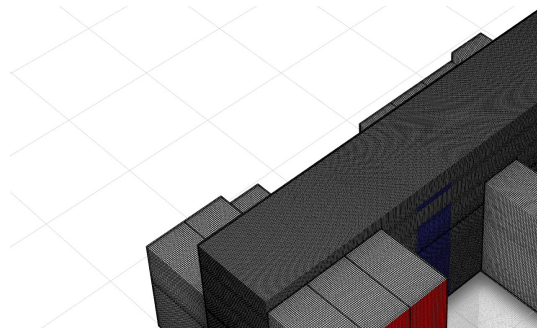
**Keywords:** CFD, Data Center, Grid Spacing, Non-conformal Grid

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With increasing power densities in next-generation data center equipment, Computational Fluid Dynamics (CFD) is a promising tool for identifying cooling inefficiencies to save costs and improve server reliability [1]. The accuracy of these simulations depends on grid spacing. While fine grids capture flow characteristics more accurately, their heavy computational demands render them impractical in large-scale simulations. Therefore, determining suitable grid spacing is the key to balancing simulation accuracy and computational demands [2].

In this preliminary work, we explored the extent of simulation accuracy which gains from grid refinement. Here, we investigated the effect of grid spacing on data center simulation results using a steady-state pressure-based SIMPLEC solver. To determine the effect of the proposed method, we performed two near-constant refinements on a uniform grid and assessed spatial convergence with Roache's Grid Convergence Index [3]. The relative errors of each grid were calculated based on values obtained by Richardson extrapolation [4]. A non-conformal grid was created with spacing informed by the uniform grid error data.

Our preliminary results suggest that uniform, locally-coarsened non-conformal grids produce results comparable to conformal grids with similar minimum spacing. A further study would involve assessing potential efficiency gains from non-uniform grids by performing unidirectional coarsening.



**Figure 1.** Non-conformal cold-aisle data center grid with localized refinement.

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## BIO-O-01

# Utilizing temperature and relative humidity data in forest restoration's success evaluation

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### ABSTRACT

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**Keywords:** *Forest restoration, Data logger, Weather data*

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Forest restoration program has performed at Mae Sa Valley, Chiang Mai for more than 20 years. However, only few studies about the restoration's success were done in this site. In this study, we evaluated the success of tropical montane forest restoration using temperature and relative humidity data. For this purpose, data loggers were installed in three different plantations: natural regeneration site, restoration plantation, and community area. Although all three plantations have similar time series data pattern, but natural regeneration site and restoration plantation can be distinguished from community area by histogram and correlation analysis results. In conclusion, our method can be used as an aspect to evaluate the success of forest restoration program.

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## BIO-O-02

### Molecular Dynamics and Virtual Screening Study for MCR-3 Inhibitors

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#### ABSTRACT

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**Keywords:** *Mobile colistin resistance, Colistin, Pyrazolone, Molecular dynamics, Screening*

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The polymixin colistin is a last line antibiotic against extensively-resistant Gram-negative bacteria for dangerous type of superbug which was used to treat multidrug resistance. The positively charged colistin bound to negatively charged lipid A can disrupt the Gram-negative bacteria outer cell membrane. To against with colistin, mobile colistin resistance gene (*mcr* gene) which is a plasmid-mediated colistin resistance mechanism has been reported that MCR acts as phosphoethanolamine (PEA) transfer reaction to lipid A on the Gram-negative bacterial outer membrane which neutralizes the negative charge on bacterial membrane and reduces the colistin binding. This consequently causes the bacteria resistance to colistin. In this study, *mcr-3* gene isolated pathogenic *Escherichia coli* strains from pig affect to efficiency of colistin. Molecular dynamic simulation showed H380 and H463 with different protonation state have effect with water accessibility. For screening test, only 8 µg/ml of the parazolone derivative compounds combine with colistin can reduce 50% colistin concentration in strain containing *mcr-3* gene comparing with strain without *mcr-3* gene. Their docking results show sharing residue interaction. Especially, T277 as a donor atom for phosphate oxygen of PEA (MCR-3 substrate). Blocking pore in the active site by pyrazolone compounds with having T277 interaction could be able to inhibit MCR-3 function.

## BIO-O-03

# Development of a Genetically Integrated PBPK Model for Predicting Uric Acid Homeostasis in Humans

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## ABSTRACT

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**Keywords:** *Physiologically based pharmacokinetic modeling, Single nucleotide polymorphism, Uric acid homeostasis*

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Uric acid is one of the vital components that ensure the proper function of our body. Serum uric acid balance is regulated mainly by the secretion and reabsorption by the kidneys. However, much of this process is still hard to accurately simulate. Particularly, genetic variation that can affect uric acid homeostasis [1] has not been incorporated into the modeling of the human kidneys before. Here, we have developed a system of equations to study the human uric acid homeostasis using the physiologically based pharmacokinetic (PBPK) model. The PBPK model incorporates blood flow and tissue composition of organs to describe how uric acid is distributed within the body. We have also implemented the concept of sub-compartments within the kidneys [2] that allows the model to incorporate the genetics of individual patients. We chose to model patients with single nucleotide polymorphisms (SNPs) on the *SLC2A9* gene because the gene variation directly affects the amount of uric acid excreted and reabsorbed by the kidneys [3]. The end product of this research can result in a framework for implementing genetic values as a subsystem while giving way to a better representation of human physiology in highly complex systems.

## BIO-O-04

# Can SARS-CoV Neutralizing Antibodies Repurpose to SARS-CoV-2 Infection?

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## ABSTRACT

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**Keyword:** COVID-19, SARS-CoV-2, neutralising antibody, MD simulation, binding free energy calculation

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The current pandemic crisis caused by a novel severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) infection has received significant attention worldwide. The treatment by drug, Remdesivir is currently the only antiviral drug that is approved by the FDA for the treatment of COVID-19 and others antiviral drugs are recommended by COVID-19 Treatment Guidelines Panel (the Panel). Moreover, WHO also recommends vaccines for emergency use such as the Pfizer/BioNTech vaccine and AstraZeneca/Oxford-developed vaccines. The antibody-mediated humoral response is crucial for preventing viral infections. In this study, the previously reported neutralising antibodies to SARS-CoV, including m396, 80R, F26G19, and S230 were chosen to investigate their function as neutralising antibodies to SARS-CoV-2. The binding interactions of protein-protein complexes were explored using all-atom molecular dynamics (MD) simulations and solvated interaction energy-based binding free energy ( $\Delta G_{\text{bind}}$ ) calculations. In comparison to CR3022 of SARS-CoV-2 neutralising antibodies, m396 and 80R were given lower  $\Delta G_{\text{bind}}$  than CR3022, the different values were 0.77 kcal/mol and 0.62 kcal/mol, respectively. So, neutralising antibodies m396 and 80R might be able to bind to the SARS-CoV-2 receptor binding domain (RBD) better than the remaining studied antibodies and CR3022. This may be suggested that neutralising antibodies of SARS-CoV can act as neutralising antibodies to SARS-CoV-2. Therefore, the obtained information can be useful for further design of novel neutralising antibodies, which are crucial for vaccine-mediated protection against viral infection and ultimately reverse the pandemic.

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## BIO-O-05

### Claudin-1 as a target for treatment of colorectal cancer

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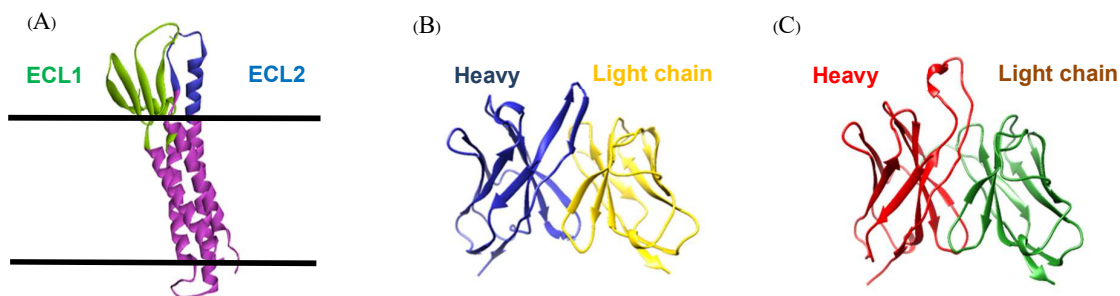
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#### ABSTRACT

**Keywords:** metastatic colorectal cancer, Claudin-1, antibody, molecular dynamics simulation

Metastatic colorectal cancer (mCRC) is a major cause of cancer-related deaths. To inhibit cancer progression, targeted therapies is used to directly inhibit molecules involving in tumorigenesis. Claudin-1 (CLDN1, Fig. 1A) is one of the attractive molecular targets for cancer therapy. It is overexpressed in several types of cancers, especially colorectal cancer (CRC). Monoclonal antibodies (mAbs) are one of the fastest-growing sector of biopharmaceutical industry and have been widely used as a therapeutic agent for the treatment of cancers and autoimmune diseases. In this study, the two mAbs against extracellular domain of CLDN1, 3A2 and 6F6 (Fig. 1B and Fig. 1C, respectively) [1, 2], were theoretically investigated by molecular docking and molecular dynamics simulation in order to evaluate the antibodies-antigen binding behaviour. As a result, both mAbs preferentially bound to extracellular loop (ECL) 1 and extracellular loop (ECL) 2 of CLDN1. Docking results base on ZDOCK scoring function in ZDOCK, revealed that 6F6 exhibited the higher docking score than 3A2 toward CLDN1. From 100 ns MD simulations of 3A2/CLDN1 and 6F6/CLDN1 complex, 6F6/CLDN1 showed the lower binding free energy than 3A2/CLDN1 similar to the result of molecular docking. At the 6F6/CLDN1 interface, there are 4 key mAb residues, including P14, T87, S88 and V121 and 5 key residues of CLDN1, including Q343, M347, I350, R387 and F395. In summary, the *in silico* results suggested that 6F6 can serve as a candidate effective anti-CLDN1 monoclonal antibody to inhibit mCRC.



**Figure 1.** Structure of (A) claudin1, (B) 3A2 mAb and (C) 6F6 mAb

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## BIO-O-06

### Substrate binding mechanism of glycerophosphodiesterase towards organophosphate pesticides

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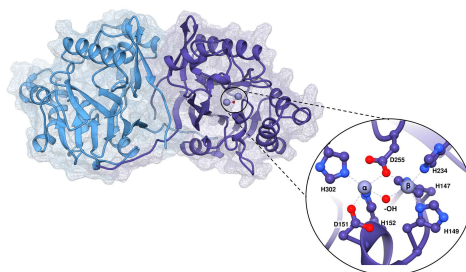
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#### ABSTRACT

**Keywords:** Methyl parathion hydrolase, organo phosphate pesticides, MD simulations

Methyl parathion hydrolase (MPH) is an enzyme from the metallo- $\beta$ -lactamase superfamily, which hydrolyses a wide range of organophosphates. MPH has attracted recent attention as a promising enzymatic bioremediator. The crystal structure of MPH enzyme shows a dimeric form, and each subunit contains a binuclear metal ion center. MPH demonstrates metal-ion-dependent selectivity patterns. The origins of this remain unclear but are linked to open questions about the more general role of metal ions in functional evolution and divergence within enzyme super families. We aimed to investigate and compare the binding of different organophosphate pesticides. For this study MPH from *Ochrobactrum sp.* was obtained and molecular docking was performed with different classes of organo phosphate pesticides such as phosphomonoester (methyl paraxon, dichlorvos), thiophosphotriester (Diazinon, Chlorpyrifos), S substituted thiophosphotriester (Profenofos), phosphorothioester (Ethion, Malathion) using Cdocker. Refined pose obtained from molecular docking was chosen for classical MD simulations using AMBER16 for 100 ns. The distance between the two Zinc metal ions were found to be stably around 3.0-3.5 Å. D255 and a hydroxyl ion acted as bridging ligand and coordinated with both the metal ions. The alpha metal ion coordinated with D151, H152, D255 and H302. It was found to be more buried and did not coordinate with the pesticide. Instead, the less buried beta metal ion was found to be coordinated with some pesticides. It was seen that the coordination of beta metal ion was perturbed to accommodate the bulky pesticides. In addition, the inhibition of the MPH enzyme by few of the carbamate and pyrethroid pesticides was also studied to understand the synergism of the pesticides. Computational studies of pesticides as opposed to the natural substrate mimics provide a better understanding due to bigger size and the formal charges involved in the pesticide. The ability of the *in-silico* analysis presented here could be informative for increasing enzyme stability and activity.



**Figure 1.** The 3D structure of homodimeric MPH, in which chain A and B are shaded by deep blue and light blue colors, respectively. The close-up regions for active site; Zn metal ions with its coordinating amino acids

## BIO-O-07

### Computational study on pyrazolopyran-based inhibitors against *Plasmodium* serine hydroxymethyltransferases

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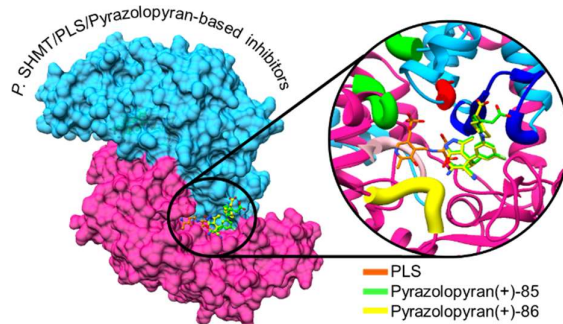
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#### ABSTRACT

**Keywords:** Serine hydroxymethyltransferase, *Plasmodium falciparum*, *Plasmodium vivax*, pyrazolopyrans, molecular dynamics, free energy calculation

Serine hydroxymethyltransferase (SHMT), one of the ubiquitous enzymes involved in one-carbon metabolism, has been considered as a promising novel antimalarial drug target due to its main catalytic function in conversion of serine and tetrahydrofolate to glycine and 5,10-methylenetetrahydrofolate, a required substrate for the de novo synthesis of purine and pyrimidine nucleotide. In this study, structural insight into the recognition of two potent pyrazolopyran-based inhibitors (pyrazolopyran(+)-85 and pyrazolopyran(+)-86) [1] in *Plasmodium* SHMTs was studied by molecular dynamics simulations for 500 ns using AMBER16 program. The results revealed that all the *Plasmodium* SHMT–inhibitor complexes remained stable during the last 100 ns, as indicated by the low fluctuation of the root-mean-square deviation and the steady number of H-bonds along the simulation time. Based on the solvated interaction energies, pyrazolopyran(+)-86 showed the stronger binding affinity towards *Plasmodium* SHMTs than pyrazolopyran(+)-85 by ~2 kcal/mol. It was better stabilized by more H-bond formations with the SHMT binding pocket residues and a lower solvent accessibility to ligand binding. Therefore, pyrazolopyran(+)-86 could be used as the template for future design and development of new antimalarial drug.



**Figure 1.** Overlay structure of pyrazolopyran-based inhibitors in *Plasmodium* SHMT.

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## BIO-O-09

### Theoretical simulations of Musashi RNA binding protein 1 in complex with target RNA

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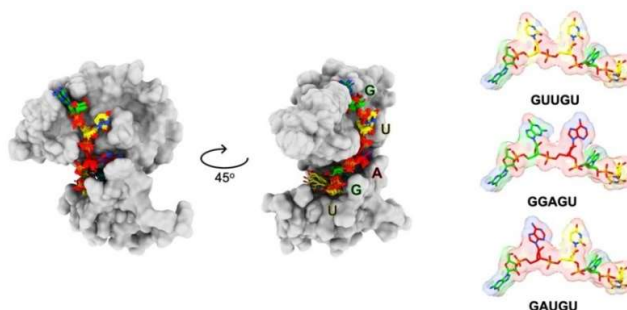
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#### ABSTRACT

**Keywords:** MSI1, RNA-binding proteins, ZIKV, MD simulation

The Musashi (MSI) family of RNA-binding proteins, comprising the two homologs Musashi-1 (MSI1) and Musashi-2 (MSI2), typically regulate translation and are involved in cell proliferation and tumorigenesis. MSI also promotes the replication of Zika virus, has triggered further investigations of the biochemical principles behind MSI-RNA interactions. In this study, various of RNA were studied by use molecular dynamics simulation. The MD simulations were performed until 100 ns and calculated the binding free energy from Poisson-Boltzmann (MM/PBSA) and generalized Born surface area (MM/GBSA) together with solvated interaction energy (SIE) suggested that GUAGU display significantly greater binding affinities than those of the three RNA (GUUGU, GGAGU and GAUGU). Several protein residues (F23, W29, R61, F63, F65, F96, R98 and R99) were involved in binding to RNA through electrostatic attractions and H-bond formations. These findings provide an in-depth understanding the interaction between MSI1-RNA.



**Figure 1** .The superimposition 20 model of Msi1-RBD1 )PDB ID :2RS2 (and three additional pentamers GUUGU, GGAGU and GAUGU

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## BIO-O-10

### Drug evaluation of darunavir analogs on the mutated HIV-1 protease

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#### ABSTRACT

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**Keywords:** Human immunodeficiency virus type-1 protease, Acquired immunodeficiency syndrome, Darunavir, HIV-1 protease inhibitors, Interaction energies

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Human immunodeficiency virus type-1 (HIV-1) protease is a successful target in the suppression of Acquired immunodeficiency syndrome (AIDS) progression by cleaving viral polyproteins contributing to mature structural and functional proteins [1]. Darunavir (DRV), approved by the Food and Drug Administration (FDA), is one of the potent HIV-1 protease inhibitors (PIs). DRV interacts with HIV-1 protease via both hydrophobic and hydrogen-bonding interactions within the active site. However, the mutations in HIV-1 protease were found to decrease DRV susceptibility [2]. In this study, we design and screen one hundred darunavir analogs in silico. The docking results showed that the top five analogs could interact with the HIV-1 protease at the active site significantly better than the darunavir. Then these analogs were investigated by 200-ns molecular dynamics simulations using the AMBER16 program. All results of the root-mean-square deviation, the steady number of H-bonds, and the binding free energies could be used to determine the potency and effectiveness of these analogs as candidates for developing PIs. The best suitable analog will be synthesized and tested with biological activity in further study.

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## BIO-O-11

# Molecular mechanism of unique interactions between APC gene and gold nanoparticles: *in silico* study for a universal cancer screening kit

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### ABSTRACT

**Keywords:** Molecular dynamics (MD) simulations, DNA methylations, Gold nanoparticles (AuNPs), Colorimetric sensor,

DNA methylation is a biological process by which methyl groups are added to the 5' position of the pyrimidine ring of cytosines. The DNA methylation profile on a promoter region of adenomatous polyposis coli (APC) gene plays a critical role in the epigenetic change that may trigger the onset of various cancers. The detection of DNA methylation on the promoter of the APC gene has become a promising candidate for early cancer diagnosis. Colorimetric sensor based on the assembly of gold nanoparticles (AuNPs) demonstrates rapid sensing and low-cost approach which can be further developed as point-of-care diagnostic tools. To gain molecular-level insights into the signature interactions between methylated DNA and AuNPs, molecular dynamics (MD) simulation was used to investigate: (i) the conformation of methylated DNA in aqueous solution; (ii) the physicochemical property of methylated DNA; (iii) physisorption of methylated DNA in the stabilization of cysteamine-capped AuNPs (Cyst/AuNPs); (iv) mechanism of DNA methylation detection via assemblies of Cyst/AuNPs. Our simulations illustrated different conformation of DNA with different methylation profile in the aqueous solution. The methylated DNA shows higher aggregation once compared with the unmethylated DNA. In the presence of Cyst/AuNPs, large aggregation of methylated DNA can prevent AuNPs from the agglomeration due to the steric hindrance. The backbone of oligonucleotides played a remarkable role in the adsorption of the DNA onto the gold surface. The oxygen, nitrogen, and methyl group in methylated DNA demonstrated non-covalent interaction between DNA and gold surface. The elucidation of adsorption of methylated DNA onto the gold surface paves the way for a novel designing of colorimetric AuNP-based biosensor for DNA methylation detection and it can be utilized as universal cancer screening.

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## BIO-O-12

### Source of oseltamivir resistance due to single E276D, R292K, and double E276D/R292K mutations in H10N4 influenza neuraminidase

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#### ABSTRACT

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**Keywords:** *Oseltamivir resistance; neuraminidase; E276D/R292K mutant; Molecular dynamics*

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Influenza is a respiratory contagious disease infecting people all around the globe. The Center for Disease Control and Prevention had estimated that from 1 October 2018 to 4 May 2019, there have been about 40 million flu patients, in which about 50 thousand cases have died. Many subtypes of influenza have developed drug resistance due to high mutation rates. Neuraminidase (NA) is the glycoprotein on the virus particle surface. Its function is to cleave the glycosidic bond with the sialic acid, leading the new virus to be able to infect other uninfected cells. Therefore, it is a promising protein target for drug design and development. The E276D and R292K NA mutations in the H10N4 influenza virus have been reported to cause drug resistance. In this study, molecular dynamics simulations and free energy calculations were applied to study the source of oseltamivir resistance in E276D, R292K, and E276D/R292K NA strains. The obtained results suggested that all studied mutants reduced the number of contact atoms, interaction energies, H-bonds, per-residue interaction energies, and total binding free energies towards the oseltamivir binding, resulting in a lower susceptibility. Only the interactions at residues 118, 119, and 371 were maintained in stabilizing the oseltamivir. The opening at 150- and 430-loops in E276D and double mutations caused the drug unbinding from the active site, increasing water accessibility into the binding pocket of NA enzyme.

## BIO-O-13

# Computational Screening of Newly Designed Compound Against Coxsackievirus A16 and Enterovirus A71

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## ABSTRACT

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**Keywords:** Hand foot and mouth disease (HFMD), Coxsackievirus A16, Enterovirus A71, Rupintrivir

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Outbreaks of hand, foot, and mouth disease (HFMD) occur around the world. It is caused by the Coxsackievirus A16 (CV-A16) and Enterovirus A71 (EV-A71) that belong to the [Enterovirus](#) genus. Unfortunately, neither an anti-HFMD drug nor a vaccine is currently available. Rupintrivir, one of drug candidates for HFMD treatment, has been attractive for the development of its analogs with board biological activities. Rupintrivir is an inhibitor for 3C protease of CV-A16 and EV-A71, an enzyme that plays a crucial role in viral replication process. *A previous study suggested that* rupintrivir analogs containing hydroxymethyl group at the P2 site showed the higher binding affinity than rupintrivir. In the present study, we aimed to search for newly designed compounds from rupintrivir analogs toward 3C protease using the Molecular Mechanics Poisson-Boltzmann or Generalized Born Surface Area (MM/PB(GB)SA) and molecular dynamic (MD) simulation approaches. From MM/PB(GB)SA calculations, our results showed that among 20 designed rupintrivir analogs there were 5 compounds (P1'-1, P2-m3, P3-4, P4-5, and P4-19) which had lower binding free energy than rupintrivir. From MD simulation analysis, P2-m3 showed stable system during the simulation for 500 ns from the RMSD value. It showed the highest number of hydrogen bond, number of contact atoms and binding free energy with 3Cpro CV-A16 and EV-A71 in the last 50-ns of the three-independent simulation. Therefore, this compound is likely to have the binding efficiency better than rupintrivir. However, druglikeness, ADMET properties, and biological testing need to be performed to ensure that this compound can serve as a more potent anti-HFMD agent.

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## CSE-O-01

### TARA: A Year in Review

**Putt Sakdhnagool<sup>1</sup>, Manaschai Kunaseth<sup>1</sup>, Apivadee Piyatumrong<sup>1</sup>, Chompoonut Rungnim<sup>1</sup>, Viwan Jarerattanachai<sup>1</sup>, Wirote Udomsiripinij<sup>1</sup>, Kittithorn Tharatipayakul<sup>2</sup>, Takdanai Suwan<sup>1</sup>, and Piyawut Srichaikul<sup>1</sup>**

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#### ABSTRACT

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**Keywords:** *Supercomputer center, Deployment, Design, High performance computing*

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In 2018, National Science and Technology Development Agency (NSTDA) has initiated a national project to establish National Science and Technology Infrastructure (NSTI) to enabling advanced scientific research and development in Thailand. As a result, the TARA cluster has been deployed and operated by NSTDA Supercomputer Center (ThaiSC) since February 2019. The cluster is a heterogeneous cluster with a theoretical peak performance of 500 teraflops. The key mission of TARA is to support large-scale computing demand from wide range of computational science applications in Thailand. In this paper, we describe the detailed cluster information and service operation of TARA cluster in the past year including the design criteria, hardware specification, management, and user support and experience. We also discuss about the challenges we encountered, and lesson learned from these experiences.

**CSE-O-02****A new algorithm with structured diagonal Hessian approximation for solving nonlinear least-squares problems and its application to robotic motion control****Aliyu Muhammed Awwal<sup>1,\*</sup>, Poom Kumam<sup>1</sup>, and Mahmoud Muhammad Yahaya<sup>1</sup>,**<sup>1</sup>*Center of Excellence in Theoretical and Computational Science (TaCS--CoE) Faculty of Science, King Mongkut's University of Technology Thonburi (KMUTT), 126 Pracha-Uthit Road, Bang Mod, Thung Khru, Bangkok 10140, Thailand*<sup>\*</sup>*E-mail: aliyumagsu@gmail.com; Tel. +66 832601605***ABSTRACT**

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**Keywords:** *iterative method; nonlinear least squares; quasi--Newton equation; motion control*

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We propose a new algorithm based on a structured diagonal Hessian approximation for solving nonlinear least-squares problems. We derived the formulation of the structured diagonal approximation of the Hessian by minimizing the deviation between the update and the previous estimate and the trace of the matrix updated so that the modified structured weak secant equation is satisfied. More so, we show the global convergence of the proposed algorithm under some standard assumptions. Comparative numerical experiments on some benchmark problems show the efficacy of the proposed algorithm. Finally, we apply the proposed algorithm to deal with robotic motion control

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## CSE-O-03

# Progressive iterative approximation method with memory and sequences of weights for least square curve fitting

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## ABSTRACT

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**Keywords:** *PIA, Least Square Curve Fitting, Sequences of Weights*

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The progressive iterative approximation method with memory and sequences of weights for least square curve fitting (SSLSPIA) is present in this paper. The method relaxes the construction of a sequence of fitting curves with the difference three real sequences of weights. Under the same assumption, and the collocation matrix is singular, its proved that these curves with appropriate alternatives of weights will converge to the solution of LSF, and that the convergence rate of the new method is faster than that of the MLSPIA method. We show some examples and applications with the efficiency and effectiveness of SSLSPIA.

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## CSE-O-04

### Derivative-free method for solving system of nonlinear equations with application

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### ABSTRACT

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**Keywords:** *Derivative-free method, spectral gradient method, Inertial effect, nonlinear monotone equations*

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Many efforts have been made to solve system of nonlinear equations due to their applications in different branches of science. Some of the early developed methods require function under consideration to be differentiable. However, not all functions representing real life applications are differentiable, thus, the methods may not be suitable in that regards. In this work, a derivative-free algorithm is proposed for solving system of nonlinear equations with convex constraint. The proposed method is derivative-free, and to accelerate the iteration process of the algorithm, inertial effect is also introduced. The global convergence of the proposed algorithm is proved under the assumptions that the mapping under consideration is Lipschitz continuous and monotone. Numerical experiments using some test problems are also presented to depict the advantages of the proposed algorithm in comparison with an existing one. Finally, the proposed algorithm is applied in signal recovery.

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## CSE-O-05

# Analysis of a Caputo HIV and Malaria Co-infection Epidemic Model

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## ABSTRACT

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**Keywords:** *Caputo fractional derivatives, Existence and uniqueness, HIV-Malaria model*

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The research aims to investigate a generalized fractional-order HIV and Malaria co-infection model. Fixed point theorems were used to investigate the existence and uniqueness of solutions to the proposed model. Numerical simulations of the modified proposed model are also conducted to demonstrate the effects. The modified fractional-order HIV and Malaria co-infection model successfully captured the trend phase of HIV and Malaria infections, providing a valuable guide for understanding the trend of the spread.

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**MST-O-01****New best proximity points theorem for generalized contraction mapping with diagonal property****W. Sanhan<sup>1</sup>, C. Phanthong<sup>2</sup> and C. Mongkolkeha<sup>1</sup>**<sup>1</sup> *Department of Mathematics Statistics and Computer Sciences, Faculty of Liberal Arts and Sciences,**Kasetsart University, Kamphaeng-Saen Campus, Nakhonpathom 73140 Thailand*<sup>2</sup> *Program of Innovation for Mathematics Instruction, Faculty of Education, Muban Chombueng Rajabhat University 70150, Thailand**\*E-mail: chirasak.m@ku.th***ABSTRACT**

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**Keywords:** *Best proximity point theorem; Diagonal property; Proximal contraction mapping*

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In this paper, we extend the concept of proximal contractions and prove new best proximity points theorems with diagonal property for such a mapping in generalized metric spaces. Also, we give some illustrative example of our main results.

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## MST-O-02

# A modification of Extragradient method without monotone mappings for solving Variational Inequality, Equilibrium and Fixed point problems

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### ABSTRACT

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**Keywords:** *Extragradient method, Nonmonotone, Armijo linesearch, Variational Inequality, Fixed point problems, Equilibrium problems*

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The propose of this work is to modify an Extragradient method (in [1]) for finding a common solution of variational inequality, equilibrium and fixed point problems without the monotone assumptions in a real Hilbert space. Weak convergence theorem is presented by the proposed method. When reducing some mappings in the method, it can find solutions of various problems without monotonicity.

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# MST-O-03

## Simpson's Second Type Integral Inequalities for Twice Differentiable Convex Functions

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### ABSTRACT

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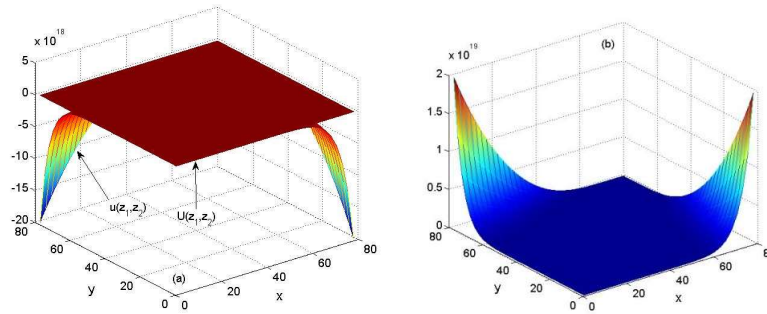
**Keywords:** Simpson's type inequality, Integral inequalities,  $\varphi$ -convex functions, Special means

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In this paper, the authors used a new auxiliary integral identity involving twice differentiable function based on a three-step quadratic kernel

$$\omega(s) = \begin{cases} \frac{s}{2} \left( \frac{1}{4} - s \right) & s \in \left( 0, \frac{1}{3} \right) \\ \frac{s}{2} (1-s) & s \in \left[ \frac{1}{3}, \frac{2}{3} \right] \\ (1-s) \left( \frac{s}{2} - \frac{3}{8} \right) & s \in \left[ \frac{2}{3}, 1 \right] \end{cases}$$

and obtained several new integral inequalities of Simpson's  $\frac{3}{8}$  type for functions whose second derivative absolute value power  $q$  are  $\varphi$ -convex and  $\varphi$ -quasiconvex function via Holder's and power mean inequality. Then we also obtain some Simpson's second type integral inequalities as special cases of our main results and also provided some applications to some special means.



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# MST-O-04

## Tseng's methods for inclusion problems on Hadamard manifolds

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### ABSTRACT

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**Keywords:** Fixed points, Hadamard manifolds, Inclusion problems, Maximal monotone vector fields, Monotone vector fields, Tseng's method

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In this article, we present two Tseng's methods for finding a singularity point of inclusion problems which is defined by means sum of single-valued vector field and multivalued vector field on a Hadamard manifold .Under standard assumptions, we prove any sequence generated by the proposed methods converges to a singularity point, whenever it exists .

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# MST-O-05

## Quantitative and Comparative Measurement of Quantum Genotype in SARS-CoV-2 and Bat Coronavirus RaTG13 With Chern-Simons Current in Genetic Code

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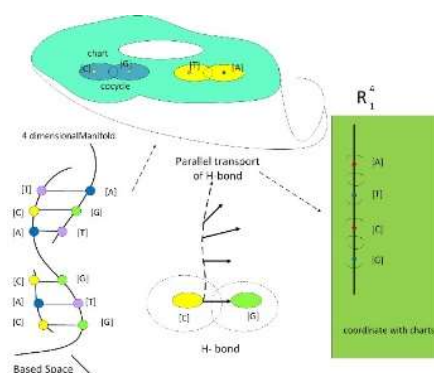
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### ABSTRACT

**Keywords:** Chern-Simons Current, Genotype, SARS-CoV-2, Bat RaTG13

The Chern-Simons current in genetic code comes from differential three from of codon triplet state with Yang-Mills field in parallel transport of coordinate system in four-dimensional model span by four bases of A, T, C, and G. It is a new methodology for empirical data analysis of plot the curvature of any protein directly from the underlying genetic code. Quantitative and comparative measurement of the quantum genotype of 29 proteins in SARS-CoV-2 was performing with Chern-Simons current using genetic code. An image of tensor correlation between 29 proteins was analyzed and constructed their hidden relationship. The plot reveals the relationship on which amino acids in SARS-CoV-2, all 29 proteins more correlated to each other. The quantitative analysis and comparative measurement of the genetic variation in E-protein of various species of coronaviruses including SARS-CoV-2 were computed by using a quantitative model based on Chern-Simons current in genetic code for finding the origin of SARS-CoV-2. The further quantum genotype comparative measurement of all genes between SARS-CoV, SARS-CoV-2, and Bat coronaviruses RaTG13 was reported. The result of empirical analysis implies that SARS-CoV-2 was evolved from Bat RaTG13 rather than SARS-CoV or other CoVs in good agree with qualitative alignment methods.



**Figure 1.** The parallel transport of coordinate system in form of chart of manifold of along the tangent space of Lagrangian of replication process of SARS-CoV-2.

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# MST-O-06

## A Novel Inertial Subgradient Extragradientt for Solving Quasi-monotone Variational Inequalities

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### ABSTRACT

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**Keywords:** *Subgradient extragradient method; Variational inequality problem; Strong convergence results; Quasi-monotone mapping; Lipschitz continuity*

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In this paper, we study the approximation solutions to variational inequalities involving quasi-monotone operators in infinite-dimensional real Hilbert spaces. We prove that the iterative sequence generated by the proposed algorithm for the solution of quasi-monotone variational inequalities converges weakly to a solution. The main advantages of the proposed iterative scheme is that it uses a monotone step size rule that depends on operator knowledge rather than its Lipschitz constant or some other line search method. Our numerical experiments are implemented to illustrate the behaviour of the new method. The numerical results have shown the effectiveness and fast convergence of the method over existing methods.

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# MST-O-07

## $\Delta$ -Convergence and Strong Convergence for Asymptotically Nonexpansive Mappings on a CAT(0) Space

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### ABSTRACT

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**Keywords:** CAT(0) Space, Asymptotically Nonexpansive Mapping,  $\Delta$ -Convergence, Strong Convergence, Fixed Point.

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In this paper, we give the  $\Delta$  and strong convergence theorems of the new three-step iteration processes for asymptotically nonexpansive mappings on a CAT(0) space. Our results extend and improve the corresponding recent results announced by many authors in the literature.

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## MST-O-08

# Hybrid LS-PRP-BFGS Like method for solving nonlinear monotone equations with applications

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### ABSTRACT

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**Keywords:** *Non-linear equations, Conjugate gradient, Projection map, Global convergence*

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A hybrid approach combined with three-term conjugate gradient (CG) method is proposed to find approximate solutions to constrained nonlinear monotone operator equations. The search direction is derived such that it is close to the memoryless Broyden-Fletcher-Goldfarb-Shanno (BFGS) direction. Without using the line search, the search direction is shown to be descent and bounded. In addition, the method converges globally under some nice assumptions. Numerical experiments are carried out on some standard test problems to test the efficiency and robustness of the method compared with existing methods. Finally, the applicability of the proposed method in other setting is considered.

## MST-O-09

Simple Poisson modules over a Poisson algebra  $S_g$ Nagornchat Chansuriya<sup>1,\*</sup> and Nongkhran Sasom<sup>2</sup><sup>1</sup>Faculty of Science, Energy and Environment, King Mongkut's University of Technology North Bangkok Rayong Campus, Rayong 21120, Thailand<sup>2</sup>Department of Mathematics Statistics and Computer, Faculty of Science, Ubon Ratchathani University, Ubonratchathani 34190, Thailand

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## ABSTRACT

**Keywords:** Poisson algebra, Poisson modules, Simple Poisson modules

Let  $S$  be a  $q$ -algebra generated by  $x, y, z, q$  and  $q^{-1}$  subject to the relations

$$xy - qyx = (q - 1)(x + y + z),$$

$$yz - qzy = (q - 1)(x + y + z),$$

$$zx - qxz = (q - 1)(x + y + z),$$

$$xq = qx, yq = qy, zq = qz, qq^{-1} = 1 = q^{-1}q.$$

We focus on a Poisson algebra  $S_q$ , constructed from  $S$ , with a Poisson brackets

$$\{x, y\} = yx + x + y + z, \{y, z\} = zy + x + y + z, \{z, x\} = xz + x + y + z. \text{ There are only two Poisson}$$

maximal ideals of  $S_q$ . In this study, we characterize the simple Poisson modules which annihilated

by each of the Poisson maximal ideals of  $S_q$ .

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# MST-O-10

## Fractal Dimension on the Difference of Thai Dance Gestures using Time Series Movement

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### ABSTRACT

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**Keywords:** *Fractal Dimension, Thai Dance Gestures, Variation Method*

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Thai dance gesture is a graceful and interpretative performance. It is closely intertwined with the beliefs, traditions and customs of Thailand and is therefore important to the lives of the people. This research aims to study the fractal dimension on the standard Thai dance gestures by the variation method of time series data. The MPO6050 Gyro sensor with Arduino is put on the right wrist for considering and analysing the data of Thai dance gestures. This research is interested in ten standard Thai dance gestures that are different rhythms. The results show that the fractal dimension of the Thai dance gestures in the slow rhythm is lower than the fast rhythm. In conclusion, the fractal dimension is an effective analysis for separating standard Thai dance gestures in the different rhythms.

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# MST-O-11

## On the existence of solutions for fractional boundary value problems on the ethane graph

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### ABSTRACT

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**Keywords:** *Fractional derivative, Fixed points, Contraction mapping, Schaefer fixed point theorem, Krasnoselskii's fixed point theorem*

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A few researchers have studied fractional differential equations on star graphs. They use star graphs because their method needs a common point which has edges with other nodes while other nodes have no edges between themselves. It is natural that we feel that this method is incomplete. Our aim is extending the method on more generalized graphs. In this work, we investigate the existence of solutions for some fractional boundary value problems on the ethane graph. In this way, we consider a graph with labeled vertices by 0 or 1, inspired by a graph representation of the chemical compound of ethane, and define fractional differential equations on each edge of this graph. Also, we provide an example to illustrate our last main result.

# MST-O-12

## Implicit Fractional Differential Equation with Nonlocal Fractional Integral Conditions

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### ABSTRACT

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**Keywords:** *Implicit fractional differential equation, Nonlocal fractional integral conditions, fixed point theorem.*

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In this paper, we study and investigate the following implicit Caputo fractional derivative and nonlocal fractional integral conditions by using Krasnosel'skii fixed-point theorem and Banach fixed point theorem. Also, we study the existence and uniqueness of this problem. An example is included to illustrate the applicability of our results.

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# MST-O-13

## Fractional-Order Delay Differential Equation with Fepanated Continuous

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### ABSTRACT

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**Keywords:** *Fractional delay differential equation, Fepanated conditions, Fixed point theorems.*

---

In this paper, we study and consider the existence and uniqueness solution of functional delay differential equation and separated condition by using the fixed point theorem of Schaefer's and Boyd-Wong non-linear condition. An example is included to illustrate the applicability of our results.

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# **MST-O-14**

## **A Finite Volume Method Solution to the 2-D Magnetotellurics Modeling Using Unstructured Quadrilateral Grids**

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### **ABSTRACT**

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**Keywords:** *2-D Magnetotelluric, Finite volume method and Mesh algorithm.*

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In this paper, a solution to the 2-D magnetotelluric (MT) modeling with the finite volume (FV) method using the unstructured quadrilateral mesh is presented. The accuracy, efficiency, and reliability of our FV forward modeling are compared and discussed. The results indicate that our FV codes provide good accuracy when the appropriate mesh is incorporated. The reliability of developed codes is also confirmed when compared to both analytical values and COMMEMI projects. In addition, our developed FV codes incorporating the unstructured quadrilateral mesh show useful and powerful features such as handling the irregular and complex subregions.

## MST-O-15

# Fixed point results Satisfying for new rational type weak contraction mappings with Applications

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### ABSTRACT

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**Keywords:** Complete metric space, fixed point, rational type contraction.

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In this talk, we give the fixed point results for new rational type weak contraction mappings in metric spaces, which are generalizations of many well-known fixed point results for several contraction types. We give some illustrative examples to show the usability of our results. As applications, we discuss the existence and uniqueness of solution for functional integral equations using our theoretical fixed point results.

**Mathematics Subject Classification:** 47H10, 54E50, 45G10.

# MST-O-16

## A New Iteration Technique for Nonlinear Operators as Concerns Convex Programming and Applicable in Signal Processing

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### ABSTRACT

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**Keywords:** *Fixed Point, Nonexpansive Retraction Mapping, Signal Processing, Convex Minimization.*

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In this research, we established a new iteration for nonexpansive retraction mapping. We show weak convergence on sequences in closed convex subset of Banach space. As applications, we apply our algorithm to solving signal processing problems.

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# MST-O-17

## Local Well-posedness of Nonlinear Time–fractional Diffusion Equation

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### ABSTRACT

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**Keywords:** *Tempered fractional calculus, Existence and uniqueness, Diffusion equation*

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We study the local well-posedness of the following time-fractional nonlinear diffusion equation

$$\begin{cases} {}^C D_{0,t}^{\alpha,\lambda} u - \Delta u = |u|^{p-1} u, & x \in \mathbb{R}^n, t > 0 \\ u(x, 0) = u_0(x), & x \in \mathbb{R}^n \end{cases}$$

where  $0 < \alpha < 1$ ,  $\lambda \geq 0$ ,  $p > 1$ ,  $u_0 \in C_0(\mathbb{R}^n)$  and  ${}^C D_{0,t}^{\alpha,\lambda}$  denotes Caputo tempered fractional derivative of order  $\alpha$ . The local existence and uniqueness results are obtained from heat kernel and fixed point theorem. Then, we extend the solution to establish a maximal mild solution. Moreover, we provide estimates for continuous dependence on initial condition.

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# MST-O-18

## On solving convex minimization problems with applications

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### ABSTRACT

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**Keywords:** *Minimization problem, Iterative method, Convex function, Game theory*

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In this paper, we introduce a modified iterative methods to solve minimization problem. Under standard relaxed conditions on the control parameters, some convergence theorems are proved. Our main result extended and improved the corresponding recent results announced by many researchers. Then we apply it to image deblurring game.

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**MST-O-19****An inertial parallel subgradient extragradient method for variational inequalities application to image recovery****Ponkamon Kitisak, Watcharaporn Chalamjiak, Damrongsak Yambangwai**

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**ABSTRACT**


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**Keyword:** *Subgradient extragradient method, Parallel algorithm, Signal recovery, Image restoration.*

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In this paper, we introduce an inertial parallel hybrid subgradient extragradient method for solving common solutions of variational inequality problems. We construct an algorithm using linesearch methods to find the unknown  $L$  constant of Lipschitz continuous mappings. A strong convergence theorem has been proved under some suitable conditions in Hilbert spaces. Moreover, we apply our proposed algorithm to image recovery and show the better efficiency of the algorithm when the number of subproblems is increasing.

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# MST-O-20

## Modified inertial parallel subgradient extragradient-line method for variational inequality problems with application to image deblurring

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### ABSTRACT

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**Keyword:** *Variational inequality, Hilbert space, Strong convergence, Image restoration, Image deblurring.*

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In this work, we propose an inertial parallel subgradient extragradient-line method to approximate a common solution of variational inequalities for L-Lipschitz continuous and monotone mappings which L is unknown. We also prove strong convergence results under some suitable conditions in Hilbert spaces. Finally, we use our proposed algorithm to solve image recovery and show that our algorithm is flexible and has good quality for use with common types of blur effects.

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# MST-O-21

## Statistical Process Control Applications for Monitoring of Volume Changes of Saltwater Fishery in Satun Province

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### ABSTRACT

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**Keywords:** CUSUM control chart, Saltwater Species

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This study was intended to investigate changes in the amount of saltwater fishery in Satun Province. From Cumulative sum control chart (2004-2016), it found that saltwater fish species is the most abundant in Satun, whereas cephalopod-crustacean, and other species were caught in the similar quantity. In addition, CUSUM indicates the abnormality occurred rapidly with less than one side of the cumulative sum  $S_i^-$  which has decreased since 2013. This sent a clear warning that the process started out of control in 2014. Therefore, CUSUM control chart can verify that the saltwater fishery in Satun province has decreased rapidly since 2013.

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## MST-O-22

# Contribution of Joule Heating and Thermal Radiation for the Flow of Powell– Eyring fluid

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### ABSTRACT

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**Keywords:** *Exponential stretching sheet, Thermal radiation, Shooting method*

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Flow in porous medium has applications in several industries mechanisms. Current research is prepared to address the transport phenomenon in hydro-magnetized flow model in porous exponential stretching sheet. Heat transport are modelled via temperature dependent models of thermal conductivity. Accordingly, the involvement of radiation, and Joule heating is considered. The flow presenting expression has been modelled via boundary layer approximation and the flow is produced due to the experimental stretching sheet. The governing equations have been approximated numerically via shooting method. The efficiency of the scheme is established by including the comparative study. Moreover, decline in velocity field is recorded against the escalating values of porosity parameter and magnetic parameter.

# MST-O-23

## Positive Solution of Boundary Value Problem Involving Fractional Pantograph Differential Equation

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### ABSTRACT

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**Keywords:** *Fractional pantograph differential equation, mixed condition, fixed point theorem.*

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In this paper, we study and integrate the positive solution of fractional pantograph differential equation with mixed conditions. The main tools for finding positive solutions of this problem are the fixed point theorems of Guo-Krasnosel'skii and Banach principle contraction. An example is included to illustrate the applicability of our results.

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# MST-O-24

## Efficient projective methods for the split feasibility problem and its applications to compressed sensing and image deblurring

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\*E-mail: prasitch2008@yahoo.com; Tel. +66 8 4373 1038

### ABSTRACT

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**Keywords:** *split feasibility problem, projection algorithm, Hilbert space, weak convergence*

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In this work, new projective algorithms using linesearch technique are proposed to solve the split feasibility problem. Weak convergence theorems are established, under suitable conditions, in a real Hilbert space. Some numerical experiments in compressed sensing and image deblurring are also provided to show its implementation and efficiency. The main results improve the corresponding results in the literature.

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# MST-O-25

## Convergence theorem for convex minimization problem in Hilbert space

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### ABSTRACT

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**Keywords:** *forward-backward method, convex minimization, convergence analysis, Hilbert space.*

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In this research, we study the convex minimization problem in the form of the sum of two proper, lower-semicontinuous and convex functions. We introduce a new forward-backward splitting algorithm. We then establish a convergence theorem under mild conditions. We give some applications of the suggested method via signal recovery. We give an analysis on parameters that are assumed in our hypothesis.

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**MST-O-26****A modified iterative method for common fixed point of Prešić nonexpansive mappings in Hadamard spaces****Kittisak Amnuaykarn<sup>1,\*</sup>, Poom Kumam<sup>1</sup>, and Nuttapol Pakkaranang<sup>1</sup>***<sup>1</sup>Department of Mathematics, Faculty of Science, King Mongkut's University of Technology Thonburi(KMUTT), 126 Pracha-Uthit Road, Bang Mod, Thung Khru, Bangkok 10140 Thailand**\*E-mail: corresponding author email; kittisak.am001@gmail.com***ABSTRACT**

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**Keywords:** *CAT(0) space, Fixed point problem, Prešić nonexpansive mappings, S-iterative method*

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In this paper, we introduce a modified S-iterative methods to approximate common fixed point of Prešić nonexpansive mappings in Hadamard spaces. Under standard relaxed conditions on the control parameters, some convergence theorems are proved. Our main result extended and improved the corresponding recent results announced by many researchers.

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# MST-O-27

## Solving the split variational inclusion problem by the inertial proximal algorithm in Hilbert Spaces

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### ABSTRACT

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**Keywords:** *split variational inclusion problem, inertial technique, linesearch, proximal algorithm, Hilbert spaces*

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In this work, we study the split variational inclusion problem (SVIP). We propose a new algorithm for solving the SVIP in the frameworks of real Hilbert spaces. We then prove its strong convergence theorem of the proposed method under suitable conditions. Finally, we give some numerical experiments to signal recovery.

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## POSTER PRESENTATION

## CHE-P-01

# Rotated Baseline Calculations for the Water Sliding Angle Measurement of a Rough Surface

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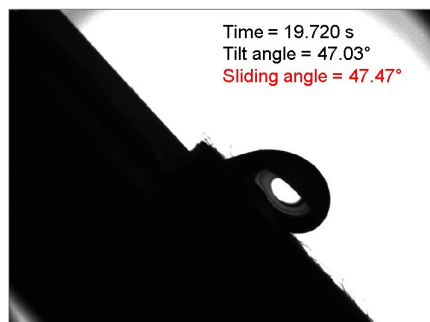
### ABSTRACT

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**Keywords:** *Water Sliding Angle, Rough Surface, Baseline, Water Repellency*

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Water sliding angle has been widely used to express the ability to repel water drops of material surface. We have recently proposed an experimental method combined with written computational scripts to estimate the water sliding angle by monitoring the rapid change of image brightness. The baseline of a flat glass surface was extracted from consecutive drop shape images, resulting the tilt angle and the corresponding rotational speed of the stage rotor. To apply this method for a rough surface such as paper, cloth, or non-woven fabric, an additional experimental setup was introduced in this work by attaching this material to a flat reference surface considered as a rotated baseline. The angular speed of the sample stage was determined by the tangent method comparing to the resulting baseline. The sliding angle was then precisely calculated by using the computer algorithms written in Matlab, which were executed to search for the frame that the water drop rolled out of the surface. It has been found that our developed experimental method and computational algorithms yielded accurate and reliable sliding angle of rough surface, thus, this method could be useful as a handy tool to study the water repellency of such advanced materials.



**Figure 1.** Water sliding angle measurement of a rough surface with corresponding tilted baseline.

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## CHE-P-02

DFT study on the effect of 3d-transition metals doping in ZnO monolayers for the CO<sub>2</sub> reduction reaction

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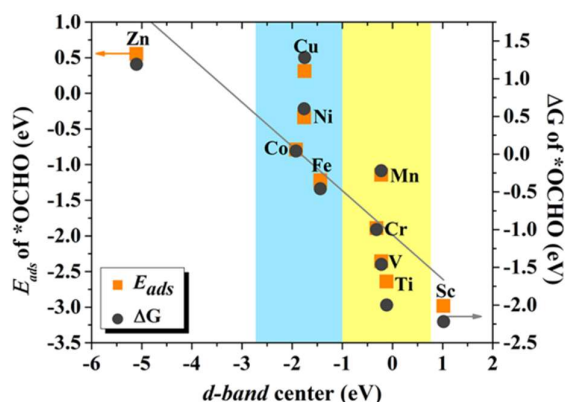
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## ABSTRACT

**Keywords:** DFT, CO<sub>2</sub> reduction reaction, ZnO monolayer, 3d doping

This work studies CO<sub>2</sub> reduction reaction (CRR) to produce C1 products on pristine and ZnO monolayers doped by 3d-transitional metal (TM-ZnO) via density functional theory (DFT) performed on the Vienna Ab initio Simulation Package code. An atom of Zn on ZnO (0001) monolayer is replaced by TM where TM is Sc, Ti, V, Cr, Mn, Fe, Co, Ni and Cu. The stability of all TM-ZnO monolayers were confirmed by the study of binding energy, cohesive energy, formation energy and Ab Initio Molecular Dynamics calculation at 500K. Different metal doping causes different CO<sub>2</sub> binding and produced different products. CO<sub>2</sub> can be reduced to HCOOH, CH<sub>3</sub>OH, and CH<sub>4</sub> depending on the TM on the TM-ZnO monolayers. Most of the TM-ZnO monolayers require smaller the overpotential for CRR compared to ZnO which requires a huge overpotential of 0.94 V. Early TMs produce CH<sub>4</sub> while late TMs produce HCOOH. Specifically, Co-ZnO requires only 0.02 and 0.45 V of overpotential for the production of HCOOH and CH<sub>3</sub>OH, respectively. Additionally, the difference in the favoured products on different surfaces can be explained by the adsorption energy ( $E_{ads}$ ) and Gibb free energy change ( $\Delta G$ ) of \*OCHO on TM-ZnO monolayer we have found in this work.



**Figure 1.** The plot of d-band center versus  $E_{ads}$  and  $\Delta G$  of \*OCHO on TM-ZnO surfaces, where Fermi level is at zero.

## CHE-P-03

# Reaction Mechanism of *n*-Pentane Aromatization over Ga Embedded H-ZSM-5 Zeolite using DFT Calculations

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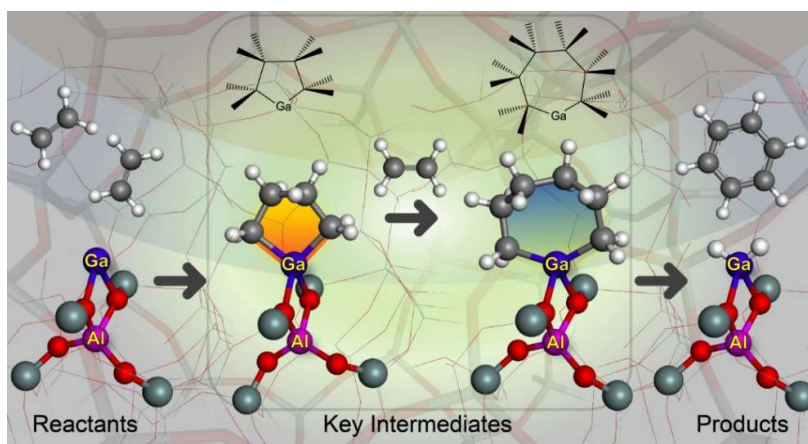
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### ABSTRACT

**Keywords:** *n*-Pentane aromatization, Ga/ZSM-5, DFT

Reaction mechanisms for *n*-pentane aromatization on Ga embedded H-ZSM-5 zeolite (Ga/ZSM-5) were elucidated using density functional theory (DFT) calculations to understand the role of Ga/ZSM-5 zeolites in aromatics synthesis. Conversion of *n*-pentane to benzene or toluene comprises four steps, i) cracking step, ii) GaH<sub>2</sub> activation step, iii) cyclization step, and iv) dehydrogenation step. Our model predicts the key intermediate in *n*-pentane aromatization on the Ga/ZSM-5 zeolite to be a five-membered Ga-C4 ring structure. The ring undergoes expansion to form a seven-membered Ga-C6 ring. The rate-determining step (RDS) for this conversion is the cyclization step of ethylene and propylene, requiring activation energies ( $E_a$ ) of 3.10 and 3.03 eV for the benzene and toluene products, respectively. Our results provide new findings for the role of Ga/ZSM-5 zeolites in *n*-pentane aromatization processes.



**Figure 1.** The key intermediate in *n*-pentane aromatization on Ga/ZSM-5 zeolite.

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## CHE-P-04

# Modelling Electron Transfer Reactions Inside Carbon Nanotubes: Molecular Dynamics Simulations

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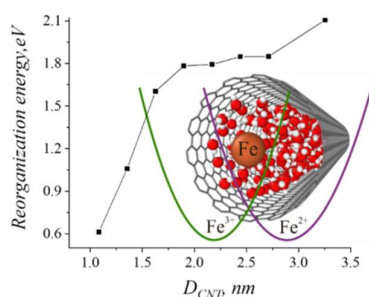
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### ABSTRACT

**Keywords:** Computational Materials Science, Molecular Dynamics Simulations, Electrochemistry, Carbon nanotubes, Redox Reactions

The structure and dynamics of electrolyte solutions inside single wall carbon nanotubes (SWCNT) are of fundamental interest. Especially, nanoconfinement effects on charge transfer processes in solutions are still scarcely studied, both experimentally and theoretical, and sometimes with contradicting results [1, 2]. We have investigated systematically the heterogeneous kinetics of a  $\text{Fe}^{3+/2+}$  redox couple in carbon nanopores in an aqueous environment. Conducting single-walled carbon nanotubes with diameters from 0.8 to 3.5 nm serve as a model of pores. Molecular dynamics simulations were performed using the LAMMPS program package [3]. The SPC/E model describes water-water while the CHARMM force field [4] and the  $\text{Fe}^{3+/2+} - \text{H}_2\text{O}$  potentials devised in Ref. [5] are used for the other interactions. We focus primarily on the solvent reorganization energy. It was calculated at several ion-wall separations by constructing two reaction free energy surfaces along the solvent coordinate. The image charge distribution was derived by solving the electrostatic problem for a perfectly conducting cylinder. Its influence on the reorganization energy is investigated. Axial and radial components of the static dielectric constant are also presented [6].



**Figure1.** Reorganization energy calculated from free energy surfaces and visualisation of the Gibbs energy surfaces for heterogeneous electron transfer along the solvent coordinate.

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# CHE-P-05

## Aldol condensation of acetone and benzaldehyde: the effect of ethanol solvent

**Mookda Meechai<sup>1</sup>, and Bundet Boekfa<sup>1,\*</sup>**

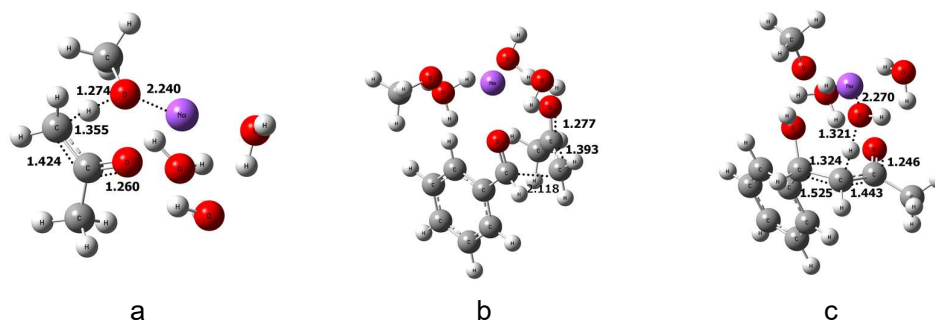
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### ABSTRACT

**Keywords:** crossed-aldol condensation, acetone, reaction rate, DFT

In this work, the crossed-aldol condensation of acetone and benzaldehyde with sodium hydroxide was investigated under a mild condition with both experiment and theory. The product was dibenzalacetone. The reaction was experimental done under optimized conditions. The reaction depends strongly on the reaction temperature. We also found that ethanol solvent is important for the reaction. Molecular-level understanding about the mechanism of aldol condensation was treated by the M06-2X Density Functional Theory (DFT). The basis set was 6-31G(d,p) level of theory. The reaction mechanism with ethoxide intermediate composed of 3 step mechanisms; tautomerization, aldol-condensation and dehydration. The total activation energies were calculated to be 11.8, 2.7 and 10.5 kcal/mol, respectively. The ethanol not only acts as a solvent to dissolve and react with each other but also improves the catalytic activity.



**Figure 1.** The optimized transition state for the crossed-aldol condensation of acetone and benzaldehyde with ethanol solvent: a) tautomerization, b) aldol-condensation and c) dehydration. Distances are in Å.

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# CHE-P-06

## Adsorption of Hydrocarbon Molecules on 2D Metal–Organic Framework $M_3HAB_2$ ( $M = Fe, Co, Ni$ and $Cu$ ) Analyzed by Frontier Molecular Orbital

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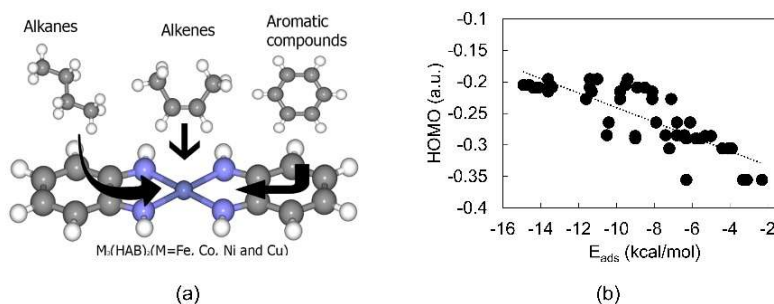
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### ABSTRACT

**Keywords:** hydrocarbon adsorption, 2D metal–organic framework, frontier molecular orbital, DFT

Adsorption is known as an important fundamental step in heterogeneous catalysis. Here, we investigated the adsorption of hydrocarbon molecules on 2D metal–organic framework  $M_3HAB_2$  ( $M = Fe, Co, Ni, Cu$  and  $HAB = \text{hexaaminobenzene}$ ) by means of the M06-L density functional theory. The 12 hydrocarbon molecules used in this work included alkanes, alkenes, and aromatic compounds. From the calculations, a linear correlation between the adsorption energies of these molecules and their highest occupied molecular orbital (HOMO) levels was observed, with an  $R^2$  value of 0.94, 0.82, 0.88 and 0.95 for  $Fe_3HAB_2$ ,  $Co_3HAB_2$ ,  $Ni_3HAB_2$  and  $Cu_3HAB_2$ , respectively. This result implied the significant role of interactions between HOMO level of the adsorbates and surface lowest-unoccupied molecular orbital (LUMO) level of the MOFs. The HOMO energies of hydrocarbons might be used as activity descriptors for an estimation of their adsorption energies.



**Figure 1.** Adsorption of hydrocarbon molecules over 2D metal–organic framework (a) and Correlations between the adsorption energies and HOMO of adsorbates (b).

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## CHE-P-07

# The mechanism of CO<sub>2</sub> hydrogenation over the Pt-decorated boron nitride nanosheets: A DFT study

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## ABSTRACT

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**Keywords:** DFT; CO<sub>2</sub> Hydrogenation; Pt-Boron nitride nanosheets; Formic acid

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The mechanism of CO<sub>2</sub> hydrogenation over the Pt-decorated boron nitride nanosheets (Pt-BNNSs) were investigated by means the density functional theory (DFT). It is found that a Pt adatom can be effectively stabilized in boron vacancy site (Pt-BV). The mechanisms of CO<sub>2</sub> hydrogenation over Pt-BV were proposed in three possible pathways: (i) co-adsorption, (ii) H<sub>2</sub> dissociation, and (iii) co-adsorption together with H<sub>2</sub> dissociation pathways. The co-adsorption together with H<sub>2</sub> dissociation provides the most favorable pathway. Our study also found that the presence of CO<sub>2</sub> in step of hydrogen dissociation plays an important role in producing the formic acid (FA) on the Pt-BV catalyst. Moreover, we found that the hydrogenation of CO<sub>2</sub> via carboxylate (COOH) has the rate-determining step of 0.63 eV in the step of hydrogen dissociation. In addition, the microkinetic modelling suggests that the COOH route is found to be more energetically and kinetically feasible rather than that it is formate route (HCOO) with the reaction temperature at 350 K and pressure of 5 bar. Our calculation results provide an important information for developing Pt-BV catalysts and might shed light on experimental design the novel Pt-BV catalyst for the CO<sub>2</sub> hydrogenation and conversion into value-added products.

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# CHE-P-08

## Density functional study of metal Lewis acid complexes Pt(PB) and Pt(PAI) for H<sub>2</sub> activation and ethylene hydrogenation

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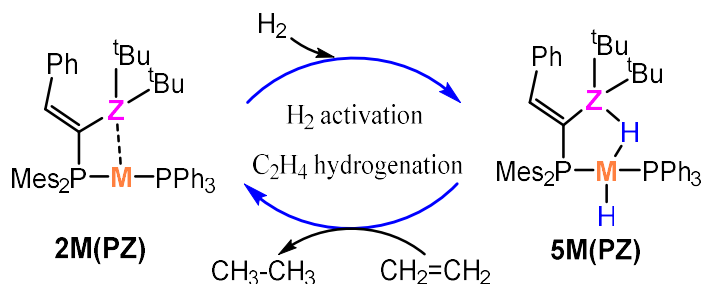
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### ABSTRACT

**Keywords:** H<sub>2</sub> activation, ethylene hydrogenation, density functional theory, platinum, nickel, Lewis acid.

The transition metal group 10 (M = Pt, Ni) can work cooperatively with the Lewis acid (Z = B, Al) towards heterolytic H<sub>2</sub> activation. Our density functional study showed that **2Pt(PAI)**, the Mes<sub>2</sub>PC(=CHPh)Al<sup>t</sup>Bu<sub>2</sub> (**PAI**) in combination with platinum metal, enables cooperative dihydrogen activation via T-shaped transition state **TS25\_PtAl** (31.6 kcal/mol), which is in accordance with the experimentally observed hydrogen activation at 80 °C.[1] We then explored the possibility of using boron instead of aluminum Lewis acid. Unlike **2Pt(PAI)**, **2Pt(PB)** has no interaction between Pt—B (3.154 Å). This allows more facile activation of dihydrogen substrate, which leads to a lower energy barrier of 21.8 kcal/mol for **2Pt(PB)**. With Ni in place of Pt, **2Ni(PB)** exhibited even higher reactivity towards H<sub>2</sub> via the tetrahedral-like transition state **TS25\_NiB** (9.7 kcal/mol). The energy required to complete the catalytic cycle for ethylene hydrogenation was calculated and used as a guide for potential reactivity of metal Lewis acid complexes.



**Figure 1.** Reaction scheme of H<sub>2</sub> activation and ethylene hydrogenation by cooperative metal-Lewis acid **M(PZ)** complexes (M = Pt, Ni ; Z = B, Al).

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# CHE-P-09

## Computational Study: The Use of Ginger-Family Plant against COVID-19 Mpro Enzyme via Molecular Docking Method

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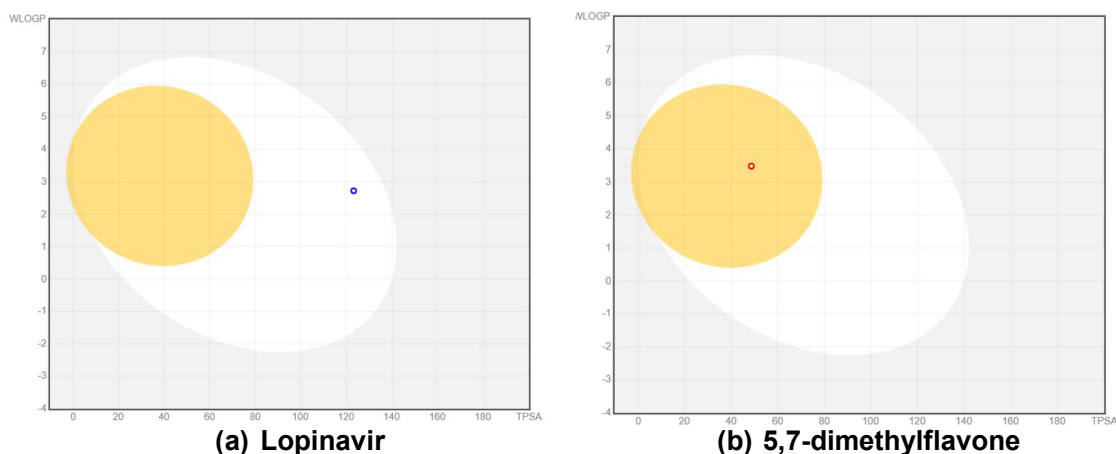
### ABSTRACT

**Keywords:** COVID-19, molecular docking, ginger

The free binding energies ( $\Delta G_{\text{bind}}$ ) of the Mpro enzyme-inhibitor were calculated using the molecular docking method. For the sake of comparison, docking lopinavir on Mpro has also been carried out. Inhibitor candidates are 4 ginger-plant compounds from black galingale, galangal and cassumunar ginger. It was found that 5,7-dimethylflavone is the studied plant-compound that has the strong binding at the active site of Mpro. It interacts to the enzyme via hydrogen bonding and hydrophobic contacts. Some physicochemical and pharmacokinetic properties were calculated and interpreted that 5,7-dimethylflavone is a druglike substance and has high gastrointestinal adsorption. This confirms that 5,7-dimethoxyflavone should be useful in formulating therapeutic strategies or used as a lead for drug development against COVID-19.

**Table 1.** Free binding energies and Mpro amino residue to which the studied plant compounds binds. Residue names expressed in red colour are those that form H-bonds to the inhibitor.

Inhibitor Candidate	( $\Delta G_{\text{bind}}$ (kcal/mol))	Enzyme amino acid residues that interact the inhibitor
lopinavir	-9.17	Thr25, Tyr54, His (41,163,164,165), Phe140, Leu (141,167), Asn142, <b>Gly143</b> , <b>Cys145</b> , Met (149,165), <b>Glu166</b> , Pro168, Asp187, <b>Gln189</b>
5,7-dimethoxyflavone	-7.76	His(41,164), Met49, Phe140, Leu141, Asn142, <b>Gly143</b> , Ser144, Cys145, Glu166, <b>His163</b> , Asp187, Arg188, Gln189
methyl cinnamate	-4.96	His(41,164), Leu141, Met49, Asn142, Phe140, Ser144, Cys145, Glu166, Asp187, Arg188, Gln189
cineole	-5.88	His41, Cys44, Met49, Pro52, Tyr54, His164, Asp187, Arg188, Gln189
sabinene	-5.10	His(41,164), Met(49,165), Tyr54, Arg188, Asp187, Gln189



**Figure 1.** BOILED-Egg diagrams: (a) lopinavir and (b) 5,7-dimethoxyflavone. The yolk is the physicochemical space for highly probable BBB permeation. The white is the physicochemical space for highly probable HIA. An active efflux from the central nervous system (CNS) or to the gastrointestinal lumen by colour-coding: blue and red dots represent for P-glycoprotein substrates and non-substrate, respectively.

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# CHE-P-10

## Adsorption of di and trihydroxybenzenes inside the UiO-66-SO<sub>3</sub>H Metal Organic Framework: An ONIOM study

Pattraporn Srirattanasakunsuk <sup>1</sup>, and Bundet Boekfa <sup>1,\*</sup>

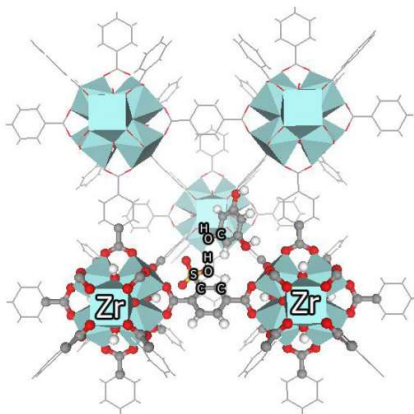
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### ABSTRACT

**Keywords:** UiO-66-SO<sub>3</sub>H, Metal Organic Framework, trihydroxylbenzenes, confinement effect

The confinement effect on the adsorption of benzene-1,3-diol, benzene-1,2,3-triol, benzene-1,2,4-triol and benzene-1,3,5-triol on the UiO-66-SO<sub>3</sub>H Metal Organic Framework (MOF) has been investigated by the ONIOM approach. The high level calculation on the functionalized benzene sulfonic with two metal node clusters was calculated with M06L/6-31G(d,p)+LANL2DZ while the lower level on the six metal node clusters was treated with PM6 calculation. To improve the adsorption energies, the optimized structures were single point calculated with M06L/6-31G(d,p)+LANL2DZ. The di and trihydroxybenzenes adsorbed inside the pore via the hydrogen bond between hydroxyl group and Brønsted acid of MOF. The adsorption energies of benzene-1,3-diol, benzene-1,2,3-triol, benzene-1,2,4-triol and benzene-1,3,5-triol on MOF were calculated to be -17.9, -23.5, -23.9 and -21.4 kcal/mol, respectively. The energy from the high level calculation were -13.4, -19.5, -18.2 and -13.2 kcal/mol, respectively. The confinement effect increase the adsorption energies up to 38% and has important implications in the synthesis of coumarin.



**Figure 1.** Benzene-1,3,5-triol adsorbed on the UiO-66-SO<sub>3</sub>H Metal Organic Framework.

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# CHE-P-11

## Molecular Dynamics Simulations on the Glass Transition Temperatures of Polyethylene terephthalate and Polyethylene vanillate

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### ABSTRACT

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**Keywords:** Polyethylene terephthalate, Polyethylene vanillate, Bio-based polymer, Glass transition temperature, Molecular dynamic simulation

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Since polyethylene terephthalate (PET) is widely used for packaging applications, the searching for an efficient way of recycling, as well as its bio-based alternatives or blending have been interested. Polyethylene vanillate (PEV) is a bio-based polymer prepared from vanillic acid and it is considered a potential alternative to PET, due to its analogous aliphatic/aromatic structures. In this study, molecular dynamics (MD) simulations of single chain polymers, PET and PEV, were applied for 50 ns using all-atom OPLS-AA forcefield. The glass transition temperatures ( $T_g$ ) of both polymers can be measured at the intersection point between the linear fitted lines. From the obtained results,  $T_g$  of PET and PEV polymers are found approximately about 349 K and 350 K, respectively. The slightly higher  $T_g$  of PEV than PET is in agreement with available experiment data. The results show that in term of  $T_g$  index, the OPLS-AA forcefield with quantum refined charges promise for using in simulations of PET, PEV and their blended polymers.

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## CHE-P-12

# Molecular Docking Studies of Berberine Derivative as Novel Multi Target PCSK9 and HMGCR Inhibitors

**Munchalika Jaitrong<sup>\*</sup>, Pornthip Boonsri, and Siritron Samosorn**

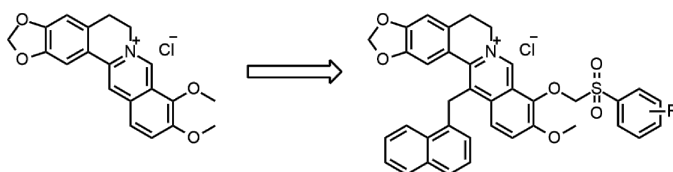
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### ABSTRACT

**Keywords:** Berberine, HMGCoA reductase, Hyperlipidemia, Multi-target directed ligands (MTDLs), Molecular docking, PCSK9

Hypercholesterolemia is a high risk for cardiovascular diseases, stroke, and mortality. Multi-target directed ligands (MTDLs) with dual inhibition of Proprotein Convertase Subtilisin/Kexin type 9 (PCSK9) and 3-hydroxy-3-methylglutaryl coenzyme A reductase (HMGCR) are the potential targets for the treatment of hyperlipidemia. In this work, a novel series of Berberine (BBR) derivatives were designed based on molecular docking to serve as MTDLs for PCSK9 and HMGCR. The binding energy of BBR derivatives was investigated, which confirmed that all the designed compounds showed better binding energy than the parent BBR for both enzymes. The effect of benzenesulfonyl ring substituent withdrawing group was /donating-with the electron .finitlyexplored to improve the binding afThe obtained results indicated that there are no significant differences in their interactions and mode of binding. Amongdesigned compounds 24 , the meta-hydroxyl substituent was identified as the most potent inhibitor due to strong interactions that were formed with Pro155, Arg194, Ala239, Ile369, Ser372, Cys378, Phe379, and Val380 of PCSK9, whereas this compound formed strong interactions with Ala525, Thr558, Gly560, Cys561, Met657, Asn658, Asp767, Gly808, Leu853, Ala856, Leu857, and His861 residues of HMGCR. Moreover, *in silico* study confirmed that all designed compounds fulfilled drug likeliness properties. Therefore, it was expected that these novels BBR derivatives could be proposed as the potential multifunctional PCSK9 and HMGCR inhibitors for hypercholesterolemia treatment.



**Scheme 1.** Design of Berberine derivatives.

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## CHE-P-13

# Machine learning-based high throughput screening of modified graphenes as electrocatalysts for CO<sub>2</sub> reduction

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## ABSTRACT

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**Keywords:** DFT, Machine learning, CO<sub>2</sub> electroreduction, electrocatalysts

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The density functional theory (DFT) has been widely used in searching catalysts for the electrochemical CO<sub>2</sub> reduction reaction (CO<sub>2</sub>RR) with a low limiting potential. However, high-throughput screening of electrocatalysts requires an expensive computational cost of DFT calculations for predicting eligible electrocatalysts. Herein, to address this issue, we combined supervised machine learning (ML) with the DFT database of various transition metal single-atom catalysts (SACs) on nitrogen-doped graphene. Besides, the heteroatoms such as boron, oxygen, nitrogen, and sulfur were incorporated to alter the structure and electronic properties of metal active sites. Overall, 207 catalysts are employed. The machine-learning model can predict the energies of the three crucial reaction steps in CO<sub>2</sub>RR; CO<sub>2</sub> adsorption energy ( $\Delta G_{\text{CO}_2}^*$ ), first protonation energy ( $\Delta G_{\text{COOH}/\text{OCHO}}^*$ ), and hydrogen adsorption energy ( $\Delta G_{\text{H}}^*$ ) of competitive hydrogen evolution reaction energy. The ML models were employed to facilitate the high-throughput screening. The models' inputs are simple elemental properties that are available in the periodic table and electronic properties from surface calculations. Using the random forest algorithm exhibited a high-level accuracy of predicted  $\Delta G_{\text{H}}^*$  and  $\Delta G_{\text{CO}_2}^*$  with a low testing root-mean-square error (RMSE) of 0.17 eV. Furthermore, the prediction of  $\Delta G_{\text{COOH}/\text{OCHO}}^*$  values via a deep neural network (DNN) presented a small number of RMSE as 0.15 eV, while the averaged R-squared value was above 0.93. The candidate electrocatalysts for CO and HCOOH productions from CO<sub>2</sub> are N4-O1-Au and N4-O1-Ag, respectively, which required potential less than 0.6 eV. The valence electron of the transition metals becomes the most important feature for the high catalytic activity of the electrocatalysts. In summary, the DFT and ML combination strategy evaluates the barrier of the key reaction step accurately and can also be a tool to identify the key feature properties that are beneficial for the rational design of electrocatalysts for CO<sub>2</sub> reduction.

# CHE-P-14

## A Mechanistic Study of the Formaldehyde Oxidation Catalyzed by MoS<sub>2</sub> Supported Single Co Atom Catalyst

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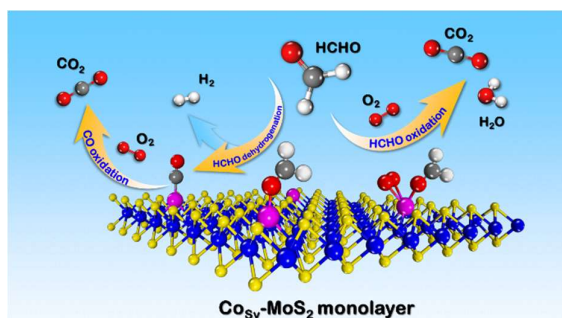
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### ABSTRACT

**Keywords:** Co-embedded monolayer MoS<sub>2</sub>; Formaldehyde oxidation; DFT

Formaldehyde (HCHO) is one of the most common toxic indoor air pollutants<sup>1</sup>. Its efficient removal at room temperature is desired. In this work, we present the complete catalytic oxidation of HCHO catalyzed by a recently synthesized single atomic catalyst (SAC)<sup>2</sup>; Co-embedded sulfur vacancy MoS<sub>2</sub> (Co<sub>SV</sub>-MoS<sub>2</sub>) monolayer, using the density functional theory calculation. The calculations demonstrate that the Co atom is strongly anchored at the S vacancy site of the MoS<sub>2</sub> monolayer forming SAC without metal clustering. From the study of all possible elementary steps, we proposed the two possible catalytic cycles for HCHO oxidation; 1) HCHO dehydrogenation route (HCHO → H<sub>2</sub> + CO) followed by CO oxidation (CO + O<sub>2</sub> → CO<sub>2</sub>), and 2) HCHO oxidation by O<sub>2</sub> route (HCHO + O<sub>2</sub> → H<sub>2</sub>O + CO<sub>2</sub>). The kinetic and thermodynamic analyses show that HCHO oxidation can take place easily on Co<sub>SV</sub>-MoS<sub>2</sub> catalyst with the energy barrier of 0.69 and 0.86 eV for the HCHO dehydrogenation and HCHO oxidation by O<sub>2</sub> routes, respectively. Therefore, non-noble metal single atom Co<sub>SV</sub>-MoS<sub>2</sub> catalyst demonstrates excellent activity for HCHO catalytic oxidation at low temperature.



**Figure 1** .Formaldehyde oxidation over Co<sub>SV</sub>-MoS<sub>2</sub> monolayer.

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# CHE-P-15

## A DFT Study on a Single Transition Metal Doped C<sub>3</sub>N for CO Oxidation Reaction

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### ABSTRACT

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**Keywords:** C<sub>3</sub>N monolayer, CO oxidation, DFT, Transition metals, LH mechanism

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The catalytic oxidation of carbon monoxide (CO) by oxygen (O<sub>2</sub>) molecule is one of the most popular methods for conversion of CO to the less toxic molecules, i.e., CO<sub>2</sub>. The C<sub>3</sub>N monolayer is an interesting catalyst for CO oxidation reactions due to its unique electronic and structural properties as well as high surface area. In this work, the adsorption of CO, O<sub>2</sub>, and CO+O<sub>2</sub> on transition metals (TM = Cu, Ni, Pt and Pd) decorated on the C, N, CC and CN vacancy of C<sub>3</sub>N monolayer are investigated by mean of density functional theory (DFT) calculations. The results show that the co-adsorption of CO+O<sub>2</sub> is more preferable than that it is CO and O<sub>2</sub> adsorption. In addition, O<sub>2</sub> is more feasibly adsorbed on surface than CO. Moreover, it is found that the gas adsorptions on Pt@Nv-C<sub>3</sub>N surface with adsorption energies (E<sub>ads</sub>) of -4.14 eV are more stable than Cu, Ni and Pd with adsorption energies (E<sub>ads</sub>) of -2.33, -3.23 and -3.30 eV respectively. According to our finding, CO oxidation on Pt@Nv-C<sub>3</sub>N surface might be occurred through the LH mechanism, starting with co-adsorption of CO and O<sub>2</sub>, then produce CO<sub>2</sub> and O\*. After that, the second CO molecule reacts with O\* to yield a second CO<sub>2</sub> molecule. Therefore, we hope that Pt doped C<sub>3</sub>N is might be a high-performance catalytic material for highly effective material for oxidative CO reaction.

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# CHE-P-16

## Computational Study of the Direct Carboxylation of Methane with Carbon Dioxide over the Metal–Organic Framework NU-1000

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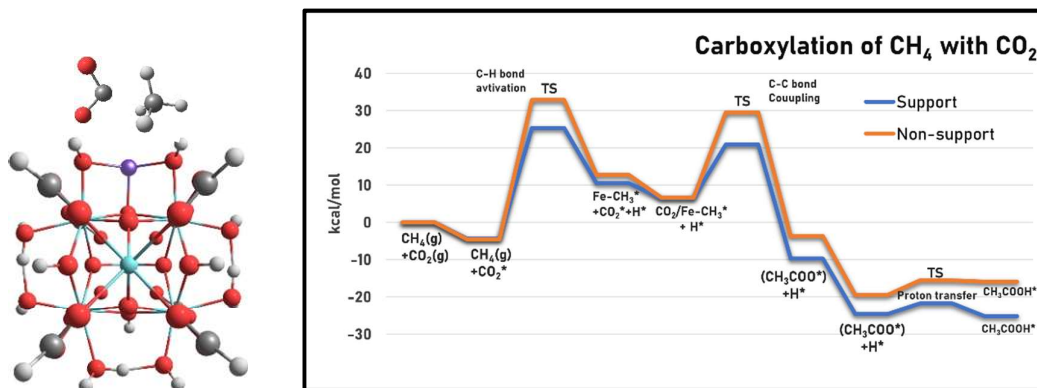
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### ABSTRACT

**Keywords:** Methane and carbon dioxide conversion, C-H bond activation, C-C bond coupling, NU-1000, DFT

The conversion of methane ( $\text{CH}_4$ ) and carbon dioxide ( $\text{CO}_2$ ) to more valuable chemicals is importance from both the environmental and industrial points of view. Here, we investigate the catalytic activity of the Fe-supported MOF NU-1000 for the direct carboxylation of  $\text{CH}_4$  with  $\text{CO}_2$  to acetic acid ( $\text{CH}_3\text{COOH}$ ) by deriving the relevant reaction profiles with density functional theory calculations. A three-step mechanism is proposed which consists of (i)  $\text{CH}_4$  C-H bond activation (ii) C-C bond coupling, and (iii) acetic acid formation. The activation of the C–H bond is the rate-determining step for the reaction which has a barrier of 29.7 kcal/mol. The effect of supported NU-1000 is also demonstrated and found to play important role since it stabilizes all species, especially the transition states leading to reducing the activation barrier by 7.7 and 8.3 kcal/mol for the  $\text{CH}_4$  C-H bond activation and C-C bond coupling, respectively.



**Figure 1** .Carboxylation of methane with carbon dioxide over the metal–organic framework NU-1000

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## CHE-P-17

# Understanding the Performance of the Single Transition Metal on M-Decorated Nitrogen-Doped Graphene for Formic Acid Decomposition: A Theoretical Study

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## ABSTRACT

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**Keywords:** Metal decorated nitrogen-doped graphene; Density functional theory (DFT); Formic acid; Adsorption

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In this work, the catalytic adsorption of FA molecule on the metals doped nitrogen graphene (M-N<sub>4</sub>GP; M = Fe, Co, Ni, Ru, Rh, Pd and Cu) have been investigated using the cluster of M-N<sub>4</sub>GP modelled by DFT+GD3BJ calculation. It is found that all metals strongly bound to N<sub>4</sub>GP. The binding energies followed the order of Fe > Ni > Ru > Co > Rh > Pd > Cu, which are in the range of −8.50 to −4.79 eV. Fe-N<sub>4</sub>GP catalyst provides the strongest binding energy, demonstrating that it is more stable surface than others. The FA dehydrogenation mechanism in M-N<sub>4</sub>GP has been extensively investigated to understand the catalytic activity of the M-N<sub>4</sub>GP substrate. The reaction can occur through two possible reaction pathways, i.e., the reaction with formate (O-H breaking) and carboxylate (C-O breaking). The first step of understanding FA decomposition mechanism is FA adsorption. We therefore first preliminary investigated FA adsorption over M-N<sub>4</sub>GP. Our calculation results showed that the FA molecule on the Fe-N<sub>4</sub>GP has the strongest interaction with a high adsorption energy of −1.45 eV among of those catalysts, indicating that Fe-N<sub>4</sub>GP can be considered as a candidate catalyst for the FA decomposition reaction.

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## CHE-P-18

# Ti<sub>4</sub>-Decorated B/N-Doped Graphene as High-Capacity Hydrogen Storage Material: A DFT Mechanistic Study

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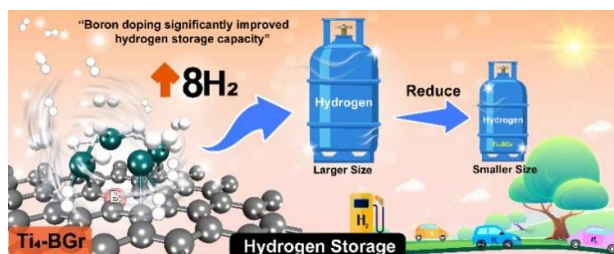
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## ABSTRACT

**Keywords:** Density functional theory, Hydrogen storage, B- and N-doped graphene, Titanium, Graphene

We perform density functional theory (DFT) calculations to investigate the hydrogen adsorption and storage on Ti<sub>4</sub> decorated on pristine, B- and N-doped graphene sheets. According to our calculations, the doping B atom on graphene could improve the interaction between the Ti<sub>4</sub> cluster and the supporting substrate. The doping of B atom on graphene has a very strong binding energy of -6.45 eV, which is the strongest interaction among of three catalysts. Additionally, the first H<sub>2</sub> molecule is likely to be dissociative chemisorption in all the substrates. PDOS analysis confirmed that the metal hydrides are preferentially found by the strong orbital hybridization between Ti-3d orbital and H-1s orbital. Furthermore, Ti<sub>4</sub> decorated B-graphene is most effective, with high capacity of hydrogen adsorptions which could be released under practical conditions. We confirmed that eight H<sub>2</sub> molecules could stably adsorb on Ti<sub>4</sub>/BGr with six reversible hydrogen adsorptions. It is evident that B-doped graphene can be enhanced the strength of adsorption between the H<sub>2</sub> molecule and the substrate. Our proposed B-doped graphene, Ti<sub>4</sub>/BGr can be considered as a high potential capacity and high-stability of hydrogen storage medium. Consequently, the Ti<sub>4</sub> decorated B-graphene is a promising candidate material for reversible hydrogen storage material.



**Figure 1.** Ti<sub>4</sub> decorated B-doped graphene as high-capacity hydrogen storage material.

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# PFD-P-01

## Extremely localized basis functions for band structure calculations and an approximated case: Finite difference approximation

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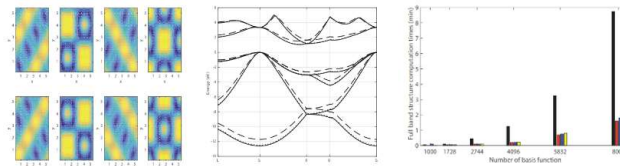
### ABSTRACT

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**Keywords:** Dirac delta function, basis function, variational method, group IV semiconductors

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In this work the Dirac delta comb function is used as a basis function to approximate the full wave function in the variational method. The validity of using this basis function was tested by calculating the electronic band structure of silicon (Si), germanium (Ge) and  $\alpha$ -tin (Sn) in diamond structure (having 8 atoms in cubic unit cell), using the modified Falicov type of atomic formfunctions. The kinetic energy term of the Hamiltonian was approximated by the second order central finite difference method, which makes the Hamiltonian matrix identical to that obtained by conventional finite difference method, which shows the identity of the two approaches. The computation time per one k-point in the band structure diagram by using 3024 basis functions with the Dirac delta function basis is smaller than with the plane waves basis, e.g. requiring 0.293, 0.206 and 0.28 minutes for the full band structure when using finite difference approximations with the order of accuracy of  $\Delta^2$ ,  $\Delta^4$ , and  $\Delta^6$ , respectively, compared to 0.48 minutes with the plane wave basis, which is widely used in electronic structure codes, making the  $\Delta^4$  finite difference accuracy with the Dirac delta basis the most efficient choice. Furthermore, the Dirac delta function basis shows their method with scales as  $O(n)$ , while the plane wave approach should scale as  $O(n \log n)$  and with the complexity of the fast Fourier transform.



**Figure 1.** (Top left) The potential in real space in silicon unit cell, (Top right) the energy band structure of silicon calculated with plane waves basis (solid), and with the Dirac delta functions basis with the finite difference approximation, and (bottom) the full energy band structure computation time, calculated with the plane waves basis (black) and with the Dirac delta functions basis with the finite difference approximation.

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# BIO-P-01

## Free Energy Calculations of Melatonin Permeation through Niosome Bilayers: A Molecular Dynamics Study

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### ABSTRACT

**Keywords:** Melatonin, Cholesterol, Span60, Potential of mean force

Molecular permeation through lipid membranes is a fundamental biological process that is important for small neutral molecules and drug molecules. Niosomes are vesicular systems comprising of bilayer made up of non-ionic surfactants such as Span60 (sorbitan monostearate) with cholesterol inclusion. They have been promoted as an excellent carrier for encapsulating both hydrophilic and lipophilic drugs. In this work, we have investigated the permeation of melatonin drug through niosome bilayers using molecular dynamics simulation. The permeation of melatonin through niosome bilayers with the addition of 0, 25, and 50 mol% cholesterol has been investigated by using the free energy calculations via the potential of mean force (PMF) method. The umbrella sampling technique was employed to the PMF calculations. The results showed that the free energy barrier of niosome bilayers decreased with cholesterol addition. The free energy barrier of the niosome bilayer with 50 mol% cholesterol is lower than the others, suggesting that the translocation of melatonin through the membrane is faster. Additionally, it can be observed that melatonin preferred to locate at the hydrophilic region (the head group of Span60). Therefore, the niosome bilayer with 50 mol% cholesterol inclusion exhibited the highest permeability, leading to easier translocation of melatonin through the membrane. The addition of cholesterol into the niosome bilayers significantly influences not only the permeability of melatonin molecule but also the bilayer structure.

**Table 1.** The free energy profiles of melatonin calculated by potential of mean force with 0, 25, and 50 mol% cholesterol.

Model	position of minimum (nm)	$\Delta G_{\text{water}}$ (kJ/mol)	$\Delta G_{\text{pen}}$ (kJ/mol)
spa_chol(0:0)	3.00	19.56	143.65
spa_chol(75:25)	2.91	25.84	91.52
spa_chol(50:50)	2.21	37.44	49.02

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## BIO-P-02

### Computational study of N501Y mutation in receptor binding domain of SARS-CoV-2 spike protein binding to human angiotensin-converting enzyme 2 receptor

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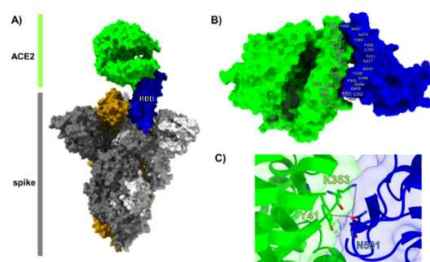
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#### ABSTRACT

**Keywords:** SARS-CoV-2; N501Y mutation, S protein RBD, ACE2, MD simulation

The recent N501Y mutation in the receptor binding domains (RBD) of SARS-CoV-2 spike protein has been reported to increase its binding efficiency to the human angiotensin-converting enzyme 2 (ACE2) receptor. Clearly, the spread of N501Y SARS-CoV-2 has increased dramatically and continuously compared to WT. The RBD binding with ACE2 (figure 1) is the one of important key of increasing new spread of SARS-CoV-2 [1]. In this study, the molecular structural and energetic properties of wild-type (WT) and N501Y SARS-CoV-2 complexed with ACE2 were studied using molecular dynamics (MD) simulations and binding free energy based on solvated interaction energy (SIE) method. The obtained results revealed that the binding affinity toward ACE 2 of N501Y RBD was higher than that of WT RBD, consistent well with the lower water accessibility at the protein-protein interface and the higher compactness of N501Y RBD/ACE 2 complex, driven by a formation of  $\pi$ - $\pi$  interaction (Y-501Y(41). In addition, the increased susceptibility of hot-spot residues of N501Y RBD was promoted by the formation of H-bonds and contacting atoms. Altogether, the N501Y enhances affinity of the prefusion state on the membrane during the fusion machinery in human. The obtained results could be helpful for the design of novel vaccines.



**Figure 1.** (A) Crystal structure of SARS-CoV-2 RBD (blue, open form) bound to the ACE2 (green) receptor (PDB ID 7A94). (B) RBD binding with ACE2 complex. (C) interaction between N501 residue of RBD and K353 and Y41 residues of ACE2.

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## BIO-P-03

***In silico* and *in vitro* studies on inclusion complexation of anthraquinone derivatives with  $\beta$ -cyclodextrin derivatives****Amy Oo<sup>1</sup>, Panupong Mahalapbutr<sup>2</sup> and Thanyada Rungrotmongkol<sup>1,3,4,\*</sup>**<sup>1</sup> *Structural and Computational Biology Research Unit, Department of Biochemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand; amyoo.educare@gmail.com*<sup>2</sup> *Department of Biochemistry, Faculty of Medicine, Khon Kaen University, Khon Kaen, 4002, Thailand; panupma@kku.ac.th*<sup>3</sup> *Ph.D. Program in Bioinformatics and Computational Biology, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand; t.rungrotmongkol@gmail.com \**<sup>4</sup> *Molecular Sensory Science Center, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand; t.rungrotmongkol@gmail.com \***\* E-mail: t.rungrotmongkol@gmail.com; Tel. +(66) 2218-5426***ABSTRACT****Keywords:**  $\beta$ -cyclodextrin; inclusion complex; anthraquinones; emodin; molecular dynamics simulation; cytotoxicity; lung cancer.

An enormous amount of research, ranging from co-solvency to nano-crystallization [1], has been carried out to enhance the water solubility of poorly soluble drugs. Out of ample techniques, complexation with  $\beta$ -cyclodextrin ( $\beta$ CD) has gained a lot of research attention due to its unique structure where many kinds of lipophilic guest molecules are entrapped into its hydrophobic cavity [2]. Anthraquinones, an important class of organic compounds prevalent in nature, have been employed as natural dyes, laxatives, and herbalism historically to chemotherapeutic agents nowadays. In this study, we investigated the cytotoxicity of 6 anthraquinones (Ventilanon K, Emodin, Chrysophanol, Aurantio-Obtusin, 1-O-methyl-2-methoxychrysophanol, and Questin) toward A549 human lung cancer cell line. Notably, Emodin (6-methyl-1,3,8-trihydroxyanthraquinone) exerted the most potent cytotoxic effect with  $IC_{50}$  value of  $34.27 \pm 1.27 \mu M$ . The anti-cancer activities of Emodin via DNA intercalation, cell cycle arrest and apoptosis [3] have been well reported. However, its usage in pharmaceutical applications has been restricted due to its poor aqueous solubility. To address this issue, we performed a series of complexation of Emodin with  $\beta$ CD and its derivatives: 2-hydroxypropyl- $\beta$ -cyclodextrin (HP- $\beta$ CD), and 2,6-di-O-methyl- $\beta$ -cyclodextrin (DM- $\beta$ CD), to identify the most promising drug carrier with regards to water solubility enhancement and augmented biological properties through host-guest complexation by *in silico* study: molecular docking, all-atom molecular dynamics (MD) simulations and binding free energy calculations via molecular mechanics/Poisson-Boltzmann (generalized Born) surface area (MM/PB(GB)SA) and *in vitro* study: cytotoxicity (MTT) assay, and phase solubility analysis. Our findings suggest that HP $\beta$ CD could be utilized as the most feasible host molecule for Emodin, with  $\Delta G_{bind, MM/GBSA}$  value of  $-4.13 \pm 4.27$  kcal/mol and 1:1 host-guest stoichiometry with stability constant ( $K_s$ ) value of  $1681 \pm 2.74 M^{-1}$  at 37°C, respectively.

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## BIO-P-04

# Computational screening of next-generation Epidermal growth factor receptor tyrosine kinase inhibitors

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## ABSTRACT

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**Keywords:** *furopyridines, EGFR-TK, molecular docking, molecular dynamics simulation, anticancer drug screening*

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Epidermal Growth Factor Receptor (EGFR) is one of four transmembrane proteins that plays an important role in cellular signaling pathways [1]. EGFR mutations have been linked specifically to non-small cell lung cancer [2]. EGFR kinase inhibitors are classified into several generations such as osimertinib, which is the third generation inhibitor [3]. This drug indicated potent activity against mutant forms and nominal activity with wild-type EGFR (EGFR-WT) [4]. After long-term clinical treatment with osimertinib, 40% of patients developed to T790M/L858R/C797S mutation (EGFR-TM). Therefore, the screening for new potent compounds against both EGFR-WT and EGFR-TM is necessary. In this study, the furopyridine compounds were elucidated using molecular docking, molecular dynamics simulations and free energy calculation based on the solvated interaction energy (SIE) method. The obtained results revealed that the seven screened furopyridine compounds showed binding ability with both EGFR-WT and EGFR-TM better than osimertinib. From SIE method, compound PD13 shows the highest binding affinity with  $\Delta G_{\text{bind}}$  value of  $-11.81 \pm 0.03$  kcal/mol and  $-9.70 \pm 0.02$  kcal/mol for EGFR-WT and EGFR-TM, respectively, which is greater than osimertinib ( $-8.51 \pm 0.03$  kcal/mol). The obtained information suggests that compound PD13 could be served as a new candidate for further developing an anti-cancer drug.

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## BIO-P-05

# Temperature effect on the structure and dynamics of melatonin inside niosome bilayers: A molecular dynamics approach

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## ABSTRACT

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**Keywords:** Melatonin; Niosomes; Entrapment; Coarse-grained, Drug Delivery

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The structural properties and dynamics of melatonin inserted into niosome bilayers have been studied by using coarse-grained molecular dynamic simulations. The simulations with temperatures varying from 27°C to 67 °C have been carried out to investigate on temperature dependence of the bilayer structure and melatonin entrapment. The simulation results revealed that the area per lipid increased while the bilayer thickness decreased with temperature increasing. Furthermore, more melatonin molecules trended to move into the bulk water at the high temperature. However, they remained inside into the bilayer at the moderate temperatures. Cholesterol additive plays a major role in the entrapment of melatonin that inserted into the niosome bilayer. Increasing the temperature caused the phase transition of niosome bilayer from the gel to liquid-ordered phases. At the lower temperature the niosome bilayer with melatonin inclusion was in the gel phase while the higher temperature it was in the liquid-ordered phase.

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## BIO-P-06

# Lomitapide, a Lipid-Lowering Agent May Have Clinical Significance Towards the Cure of P38 $\alpha$ MAPK-Related Diseases

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## ABSTRACT

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**Keywords:** MAPK, P38 $\alpha$ -MAPK, Drug Repositioning, Molecular Docking, *In silico* screening

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P38 $\alpha$  mitogen-activated protein kinase (p38 $\alpha$  MAPK), one of the p38 MAPK isoforms participating in a signalling cascade, has been identified its pivotal role with the regulation upon great deals of physiological processes such as cell proliferation, differentiation, survival and death [1]. With biological proven evidences, enormous efforts have been collectively putting onto searching effective drugs for the reason that it could be a promising strategy for the management of cancer, neurodegeneration, and inflammatory diseases. Here, with shedding light on the advancement of computational biology contributed to the pre-clinical stage of drug discovery and development, we found that Lomitapide approved to use as pharmacological therapy in patients with homozygous familial hypercholesterolemia (HoFH) [2] could be able to act as a potent inhibitor targeting p38 $\alpha$  MAPK. *In silico* results revealed that Lomitapide has greater binding patterns and characteristics when compared to BIRB796 (a well-known p38 $\alpha$  MAPK inhibitor). Binding energy predicted from both molecular docking and solvated interaction energy (SIE) approaches exhibited a significant lower value than BIRB796 indicating an enormous greater binding capability towards the binding-site cleft. Specifically, we found that Van der Waals interaction energy was the main force driven the formation of the enzyme-drug-like complex. In addition, some other parameters were found to be corresponding with the higher magnitude of Lomitapide binding recognition. For instance, non-covalent contacts of any atoms counted within the 5.0 Å sphere of the ligand were quantitatively higher, which tends to have greater intermolecular interactions whereas the surface area occupied by water molecules termed SASA showed a gradual lower value compared to a reference complex. Thus, for the lines of evidence regarding the computational results, Lomitapide could become a viable candidate for further investigation necessary for guiding its clinical significance towards the therapeutic potentials of p38 $\alpha$  MAPK-related diseases.

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# KPS-P-01

## Green Synthesis of Selenium Nanoparticles using *Phyllanthus emblica* Fruit Extract and Selenium Uptake in Sunflower and Morning Glory Sprouts

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### ABSTRACT

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**Keywords:** Selenium nanoparticles, Selenium uptake, Green chemistry, *Phyllanthus emblica*, Bioavailability

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The aim of this research was to synthesize selenium nanoparticles (SeNPs) using ascorbic acid and *Phyllanthus emblica* extract as reductants. The size and morphology of SeNPs from both synthetic methods were characterized by using UV-Visible spectrophotometer, Fourier Transform Infrared Spectrometer (FT-IR) and Dynamic Light Scattering (DLS). The result showed that the spherical SeNPs, using 95% EtOH as solvent and SeNPs, using 95% EtOH:H<sub>2</sub>O (2:3 v/v) have diameter about 3069.0±825.69 nm and 180.3±10.17 nm while SeNPs which was synthesized by chemical reagent have particle size 313.9±24.47 nm. The presence of SeNPs was confirmed by UV-Visible spectroscopy for surface plasmon resonance (276 nm). The seed germination of sunflower and morning glory sprouts were also studied in term of root lengths and shoot lengths. The result showed that SeNPs using *Phyllanthus emblica* extract with a solvent as 95% EtOH has the lowest germination of sunflower sprouts while SeNPs did not affect to the germination of morning glory sprouts. The adsorption of SeNPs in morning glory sprouts was evaluated by Graphite Furnance Atomic Absorption spectroscopy (GFAAS). The result revealed that the absorption of SeNPs was not found in morning glory sprouts.

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## KPS-P-02

# Synthesis of Coumarin Derivative and Effect of Seed Coating with Biopolymer and Coumarin Derivatives on Sweet Corn and Tomato Seed Quality

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### ABSTRACT

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**Keywords:** Seed coating, 7-hydroxy-4-methyl coumarin, 4-methyl-7-stearoyl coumarin, Biopolymer, Seed quality

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The aim of this research was to synthesize a novel seed coating material, which comprised of fluorescent active compound coumarin derivatives and biopolymer poly  $\gamma$ -glutamic acid and Carboxymethylcellulose (CMC) as plasticizer. Two coumarin derivatives, 7-Hydroxy-4-Methyl-2H-Chromen-2-One (D1) and 4-Methyl-7-Stereoyl-2H-Chromen-2-One (D2) were synthesized in 73.95% and 42.42% yield, respectively. The effect of biopolymer and both of coumarin derivatives on sweet corn and tomato seed quality were also studied. The result showed that 4-Methyl-7-Stereoyl-2H-Chromen-2-One (D2) based seed coating material could promote the germination rate and the growth of tomato. Meanwhile, it has no effect on the germination and growth rate of the sweet corn seed coated with 7-Hydroxy-4-Methyl-2H-Chromen-2-One (D1) and 4-Methyl-7-Stereoyl-2H-Chromen-2-One (D2). The film coating made of 4-Methyl-7-Stereoyl-2H-Chromen-2-One (D2) was highly water-soluble (more than 66%) with a neutral pH at 7.4. In addition, The determination of coumarin derivatives D1 content after 6 months of storage at 15 and 25 °C was evaluated by high performance liquid chromatography.

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**KPS-P-03****Structures and absorbance properties of the combination of chlorophyll and anthocyanin used for dye sensitized solar cells (DSSC)****Suphanni Jaichueai and Piti Treesukol\****Chemistry Department, Faculty of Liberal Arts and Science, Kasetsart University, Kamphaeng Saen Campus, Nakhonpathom 73140 THAILAND**\*Email : faasptt@ku.ac.th***ABSTRACT****Keywords:** *DSSC, chlorophyll, anthocyanin, Density functional theory*

Recently, combinations of natural dyes, such as chlorophyll and anthocyanin, have been concerned as sensitized dyes for the dye-sensitized solar cell (DSSC). The optimum combination of dyes exhibiting the best performance was suggested as a result of synergetic effect between each dyes. However, the effect from Chlorophyll-anthocyanin interaction in UV-Vis excitation has not been discussed in molecular level. In this study, the density functional theory and time-depended DFT calculation with B3LYP functionals were utilized to examine the interaction between Chlorophyll-A and three different anthocyanins (cyanidin, malvidin and peonidin) and their effects on the UV-Vis excitations. According to the frontier orbitals analysis, the HOMO's of the dye complexes were mainly contributed by chlorophyll, which were slightly disturbed by the presence of anthocyanin. Although, only small red-shifts of the maximum-wavelength absorption were found in range of 10 nm, the number of UV-Vis adsorption excitations and the probability of UV-Vis absorption was significantly increased because of the charge re-distribution of the chlorophyll.

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## KPS-P-04

# Removal of organic solvents in water by carbon aerogels from pomelo peels

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## ABSTRACT

**Keywords:** Carbon aerogels, Adsorption

Pomelo peel is an agricultural waste material that can be used as an adsorbent and it is environment friendly. This research is to study the adsorption ability of carbon aerogels from pomelo peels to adsorb 3 organic solvents: hexane, benzene, and toluene. Results showed that the carbon aerogels adsorbed toluene ( $849.37 \pm 159.09\%$ ) as the most, following by benzene ( $748.43 \pm 62.68\%$ ) and hexane ( $477.61 \pm 52.93\%$ ), respectively. The adsorptions of the three solvents in water showed that carbon aerogels adsorbed for 20 seconds of toluene ( $719.08 \pm 73.25\%$ ) as the most, following by benzene ( $605.51 \pm 63.45\%$ ) and hexane ( $595.81 \pm 41.96\%$ ), respectively. Moreover, the study on adsorption ability of recycle carbon aerogels 20 seconds showed that percentages of adsorption of 5 recycle times were not different from the first adsorption. Therefore, carbon aerogels from pomelo peels had potential in application to remove organic solvents in water.

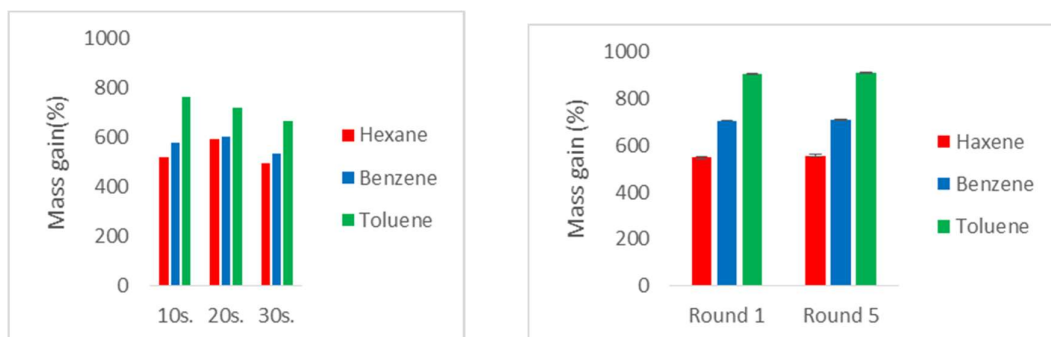


Figure 1. Adsorption of organic solvents in water by carbon aerogels produced from grapefruit peel.

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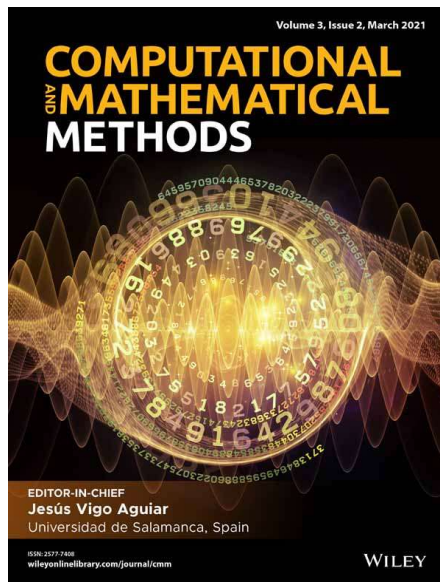
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