The 10th International Conference of the Asian Consortium on Computational Materials Science (ACCMS-10)

22-26 July 2019
City University of Hong Kong
Hong Kong SAR

Post-Conference Report

Acknowledgement
The 10th International Conference of the Asian Consortium on Computational Materials Science (ACCMS-10) was held during 22-26 July 2019 in Hong Kong. The conference was hosted by Department of Chemistry, City University of Hong Kong and supported by six local universities, including, the Chinese University of Hong Kong, Hong Kong Baptist University, the Hong Kong Polytechnic University, the University of Hong Kong, the Hong Kong University of Science and Technology, and University of Macau, with financial support from K. C. Wong Education Foundation, Prof. Yoshiyuki Kawazoe on behalf of ACCMS and TOMBO ab initio Program, Surfaces Editorial Office and also cultural activity support from Hong Kong Tourism Board.

ACCMS was established in 2000, aiming to promote international research and development in Computational Materials Sciences, particularly for Asian countries. Following the first preparatory meeting of ACCMS held in Sendai, Japan (2000), nine general international meetings had been successfully held in Bangalore, India (2001), Novosibirsk, Russia (2004), Beijing, China (2005), Seoul, South Korea (2007), Hanoi, Vietnam (2009), Biopolis, Singapore (2011), Nakhon Ratchasima, Thailand (2013), Taipei, Taiwan (2015) and Kuala Lumpur, Malaysia (2017). This year in 2019, 211 delegates from 4 continents covering 22 countries/regions came to Hong Kong to celebrate the 10th biennial-anniversary of this ACCMS international conference series.
The majority of delegates of ACCMS-10 are from Asian countries, including 25% from Hong Kong/Macau Special Administrative Regions, 18% from Mainland China, 18% from Japan, 10% from South Korea, 4-5% each from Thailand, India, Taiwan and Singapore.

Summary of Delegates Participated at ACCMS-10 in Hong Kong (2019)

The ACCMS-10 covered a wide range of scientific topics from fundamental development in theory and computational methods to various kinds of applications covering “Materials in All Forms”. The
pre-conference events included the TOMBO ab initio Program Tutorial and 4 introductory lectures for young researchers. The main scientific program consisted of 5 plenary lectures, 114 invited talks and 27 contributed talks arranged in 4 parallel sessions, and 2 poster sessions with 41 posters (including 33 poster flash talks).

The pre-conference events began with a half-day tutorial on first-principles all-electron mixed basis calculations with the TOhoku Mixed-Basis Orbitals (TOMBO) ab initio Program in the morning of 23 July 2019. The speakers were Prof. Yoshiyuki Kawazoe of Tohoku University, Prof. Kaoru Ohno of Yokohama National University and Dr. Ryoji Sahara of National Institute for Materials Science. About 50 participants attended this tutorial.

It was followed by the 4 introductory lectures for young researchers, covering general topics from as small as electrons and atoms to clusters, crystals, crystals/liquid interface, and to crystals under extreme conditions. The lectures were delivered by Prof. Yoshiyuki Kawazoe of Tohoku University (Japan), Prof. Puru Jena of Virginia Commonwealth University (USA), Prof. Enge Wang of Peking University (China) and Prof. John S. Tse of University of Saskatchewan (Canada). This educational lecture series, chaired by Prof. Gour P. Das of Indian Institute of Technology, Kharagpur (India), attracted over 130 audiences.

Prof. Yoshiyuki Kawazoe
Tohoku University, Japan
Topic: Basics and Limitations in Computational Materials Design - What we should learn before starting computer simulation –

Prof. Puru Jena
Virginia Commonwealth University, USA
Topic: From Clusters to Crystals: A Journey

Prof. Enge Wang
Peking University, China
Topic: Full Quantum Nature of Water on Salt Surface

Prof. John S. Tse
University of Saskatchewan, Canada
Topic: Computational Materials Science at Extreme Conditions

The 5 plenary lectures were delivered by Prof. Puru Jena of Virginia Commonwealth University (USA), Prof. Wenjian Liu of Shandong University (China), Dr. M. Saeed Bahramy of The University of Tokyo (Japan), Prof. Nicola Marzari of École Polytechnique Fédérale de Lausanne (Switzerland) and Prof. Su-Huai Wei of Beijing Computational Science Research Center (China). These lectures were respectively chaired by Prof. Enge Wang of Peking University (China), Dr. Kai-Chung Lau of City University of Hong Kong (HKSAR), Prof. Kwang-Ryoo Lee of Korea Institute of Science and Technology (South Korea), Dr. Patrick H.-L. Sit of City University of Hong Kong (HKSAR), and Prof. John S. Tse of University of Saskatchewan (Canada).
Prof. Puru Jena  
Virginia Commonwealth University, USA  
Topic: *Many Faces of Carbon*

Prof. Wenjian Liu  
Shandong University, China  
Topic: *The Static-Dynamic-Static Framework for Strongly Correlated Electrons*

Dr. M. Saeed Bahramy  
The University of Tokyo, Japan  
Topic: *Unraveling Emergent Quantum Phenomena Using First-principles Approaches*

Prof. Nicola Marzari  
École Polytechnique Fédérale de Lausanne, Switzerland  
Topic: *Discovering Novel Materials, and Novel Physics, with First-principles Simulations*

Prof. Su-Huai Wei  
Beijing Computational Science Research Center, China  
Topic: *First Principles Design of Materials for Energy and Optoelectronic Device Applications*

In the ACCMS-10 conference, the ACCMS Award 2019 and ACCMS Mid-career Award 2019 were presented, respectively, to Prof. Jisoon Ihm of Pohang University of Science and Technology (South Korea) and Prof. Rodion Belosludov of Tohoku University (Japan) in recognition of their outstanding scientific achievement in computational materials science research and great contribution to the ACCMS community. Supportive encouragements were also given to 11 young researchers selected based on their scientific merits contributed to ACCMS-10.
<table>
<thead>
<tr>
<th>Awards</th>
<th>Authors (the presenting authors are highlighted)</th>
<th>Institution</th>
<th>Topics</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Surfaces</strong>&lt;br&gt;Best Poster Award</td>
<td><strong>He Wen</strong>, Kanchan Ulman and Su Ying Quek</td>
<td>National University of Singapore, Singapore</td>
<td>Mechanisms for Surface-enhanced Raman Effect on Monolayer h-BN</td>
</tr>
<tr>
<td>Best Flash Talk Awards</td>
<td><strong>Jingsi Qiao</strong> and Su Ying Quek</td>
<td>National University of Singapore, Singapore</td>
<td>Charge Doping and Strain Effects on the Charge Density Wave and Superconducting Properties of H-TaS₂</td>
</tr>
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<td></td>
<td><strong>Jun Oshiki</strong>, Kento Kosugi, Hiroshi Nakano, Masahiro Higashi, and Hirofumi Sato</td>
<td>Kyoto University, Japan</td>
<td>Construction of DFTB3 parameters for platinum in an organometallic complex</td>
</tr>
<tr>
<td><strong>Kawazoe Prizes</strong> (Best Posters)</td>
<td><strong>Pooja Basera</strong>, Manish Kumar, and Saswata Bhattacharya</td>
<td>Indian Institute of Technology Delhi, India</td>
<td>Exploring the Role of N-, Mn-doping and Mn-N co-doping to Enhance the Photocatalytic Activity of SrTiO₃ Perovskite: A Hybrid Density Functional Study</td>
</tr>
<tr>
<td></td>
<td><strong>Daisuke Okamoto</strong>, Yoshihiro Watanabe, Norio Yoshida, and Haruyuki Nakano</td>
<td>Kyushu University, Japan</td>
<td>Implementation of state-averaged MCSCF method to RISM- and 3D-RISM-SCF schemes</td>
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<td><strong>R. K. Zhdanov, K. V. Gets, Y. Y. Bozhko, O. S. Subbotin, and V. R. Belosludov</strong></td>
<td>Nikolaev Institute of Inorganic Chemistry, Russia</td>
<td>Methane, Carbon Dioxide, Nitrogen Gas Hydrates Self-Preservation Effect Theoretical Study</td>
</tr>
<tr>
<td><strong>Best Contributed Talk Awards</strong></td>
<td><strong>Mehmet Emin Kilic</strong>, Aloysius Soon, and Kwang-Ryeol Lee</td>
<td>Korea Institute of Science and Technology, Korea</td>
<td>Developing a Computational Platform for Theoretical Spectroscopy of Nanomaterials</td>
</tr>
<tr>
<td></td>
<td><strong>Xiangxuan Deng</strong> and Chi-Man Lawrence Wu</td>
<td>City University of Hong Kong, Hong Kong SAR</td>
<td>Adsorption of Molecular Oxygen on Ti-doped Monolayer MoS₂ and the Effect of Strain: A DFT Study</td>
</tr>
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<td></td>
<td><strong>Shu-Hao Yeh</strong>, <strong>Aaditya Manjanath</strong>, Yuan-Chung Cheng, Jeng-Da Chai, and Chao-Ping Hsu</td>
<td>Institute of Chemistry, Academia Sinica, Taiwan</td>
<td>Excitation Energies from Thermally-Assisted-Occupation Density Functional Theory: Theory and Computational Implementation</td>
</tr>
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<td><strong>Cheng-chau Chiu</strong>, Thong Nguyen Minh Le, Amol Deshmukh, and Jer-Lai Kuo</td>
<td>Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan</td>
<td>A Computational Study on H₂ Adsorption in a Porous Framework Structure ... and the Uncertainty of its Results</td>
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<td><strong>Wai Kit Tang</strong>, Xiaoyan Mu, Ivan K. Chu, and Chi-Kit Siu</td>
<td>City University of Hong Kong, Hong Kong SAR</td>
<td>Dissociative Electron Transfer Via n→π⁺ Interaction In Isolated Tyrosine-Containing Molecular Peptide Radical Cations</td>
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*Summary of awards presented to young researchers at ACCMS-10*
The ACCMS International Advisory Committee together with representatives from ACCMS Member Countries had the Business Dinner Meeting on 24 July 2019 to review and discuss the directions of ACCMS. The members agreed to explore more Asian countries that may be interested in hosting the future ACCMS meetings. Candidate countries include Indonesia, Kazakhstan, or Philippines. The decision for the 11th ACCMS International Conference (ACCMS-11) in 2021 will be announced later.

In 5-7 February 2020, the ACCMS Theme Meeting: International Conference on Material Genome will be held at SRM University, AP-Amaravati, India, headed by Prof. D. Narayana Rao with Prof. Ranjit Thapa and Dr. Umesh Waghmare. Detailed information about this upcoming ACCMS theme meeting is available at https://srmap.edu.in/accms-2020/.

Sincerely Yours,

Dr. Chi-Kit Andy Siu, Chair
Dr. Kai-Chung Lau, Co-chair
Dr. Patrick H.-L. Sit, Co-chair

On behalf of ACCMS-10 Local Organizing Committee
August 2019