

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

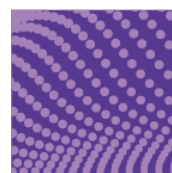


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王寬誠教育基金會
K. C. WONG EDUCATION FOUNDATION



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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.

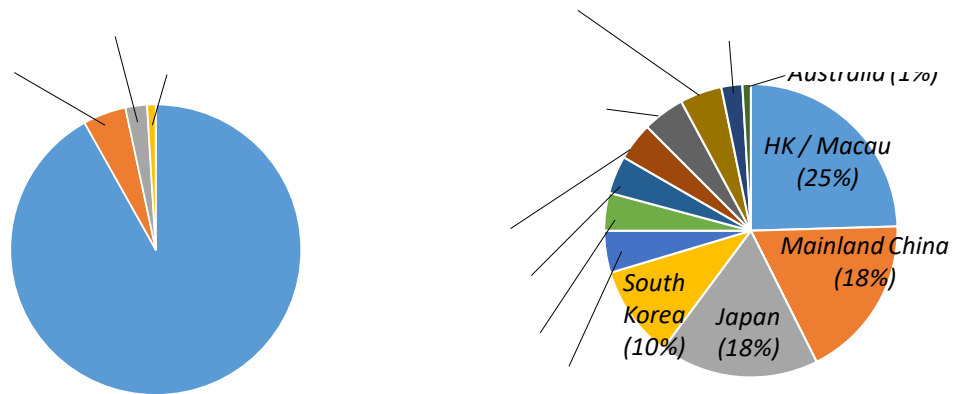


History of ACCMS Biennial International Conferences



Celebration of the 10th Biennial of ACCMS. Photo on left: Lion Dance Performance; Photo on right, Cake-cutting ceremony [from left to right: Dr. Patrick Sit, Dr. Kai-Chung Lau, Prof. Yoshiyuki Kawazoe, Dr. C.-K. Andy Siu]

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)



ACCMS-10 Group Photo Taken on 23 July 2019



ACCMS-10 Group Photo Taken on 25 July 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-Ryeo 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.



ACCMS Mid-career Award 2019 presented to Prof. Rodion Belosludov of Tohoku University, Japan



ACCMS Award 2019 presented to Prof. Jisoon Ihm of Pohang University of Science and Technology, South Korea

Awards	Authors (the presenting authors are highlighted)	Institution	Topics
Surfaces Best Poster Award	He Wen , Kanchan Ulman and Su Ying Quek	National University of Singapore, Singapore	Mechanisms for Surface-enhanced Raman Effect on Monolayer h-BN
Best Flash Talk Awards	Jingsi Qiao and Su Ying Quek	National University of Singapore, Singapore	Charge Doping and Strain Effects on the Charge Density Wave and Superconducting Properties of H-TaS ₂
	Jun Oshiki , Kento Kosugi, Hiroshi Nakano, Masahiro Higashi, and Hirofumi Sato	Kyoto University, Japan	Construction of DFTB3 parameters for platinum in an organometallic complex
Kawazoe Prizes (Best Posters)	Pooja Basera , Manish Kumar, and Saswata Bhattacharya	Indian Institute of Technology Delhi, India	Exploring the Role of N-, Mn-doping and Mn-N co-doping to Enhance the Photocatalytic Activity of SrTiO ₃ Perovskite: A Hybrid Density Functional Study
	Daisuke Okamoto , Yoshihiro Watanabe, Norio Yoshida, and Haruyuki Nakano	Kyushu University, Japan	Implementation of state-averaged MCSCF method to RISM- and 3D-RISM-SCF schemes
	R. K. Zhdanov , K. V. Gets, Y. Y. Bozhko, O. S. Subbotin, and V. R. Belosludov	Nikolaev Institute of Inorganic Chemistry, Russia	Methane, Carbon Dioxide, Nitrogen Gas Hydrates Self-Preservation Effect Theoretical Study
Best Contributed Talk Awards	Mehmet Emin Kilic , Aloysius Soon, and Kwang-Ryeol Lee	Korea Institute of Science and Technology, Korea	Developing a Computational Platform for Theoretical Spectroscopy of Nanomaterials
	Xiangxuan Deng and Chi-Man Lawrence Wu	City University of Hong Kong, Hong Kong SAR	Adsorption of Molecular Oxygen on Ti-doped Monolayer MoS ₂ and the Effect of Strain: A DFT Study
	Shu-Hao Yeh, Aaditya Manjanath , Yuan-Chung Cheng, Jeng-Da Chai, and Chao-Ping Hsu	Institute of Chemistry, Academia Sinica, Taiwan	Excitation Energies from Thermally-Assisted-Occupation Density Functional Theory: Theory and Computational Implementation
	Cheng-chau Chiu , Thong Nguyen Minh Le, Amol Deshmukh, and Jer-Lai Kuo	Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan	A Computational Study on H ₂ Adsorption in a Porous Framework Structure ... and the Uncertainty of its Results
	Wai Kit Tang , Xiaoyan Mu, Ivan K. Chu, and Chi-Kit Siu	City University of Hong Kong, Hong Kong SAR	Dissociative Electron Transfer Via n→π* Interaction In Isolated Tyrosine-Containing Molecular Peptide Radical Cations

Summary of awards presented to young researchers at ACCMS-10



ACCMS-10 Best Poster Awards presented at the conference banquet on 25 July 2019. [Photo from left to right: Prof. Yoshiyuki Kawazoe, Mr. Jun Oshiki, Mr. Daisuke Okamoto, Ms. Pooja Basera, Dr. Jingsi Qiao, Ms. Wen He, Dr. Ravil Zhdanov, Dr. C.-K. Andy Siu]



ACCMS-10 Best Contributed Talk Awards presented at the conference closing on 26 July 2019. [Photo from left to right: Dr. C.-K. Andy Siu, Dr. Wai-Kit Tang, Dr. Mehmet Emin Kilic, Dr. Aaditya Manjanath, Dr. Cheng-Chau Chiu, Dr. Patrick Sit, Dr. Kai-Chung Lau]

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