The 5th China-Japan-Korea Workshop on Theoretical and Computational Chemistry

	Jan.12 Wednesday	Jan.13 Thursday	Jan.14 Friday
9:00			
		9:30-10:20 T4(D. Cho)	9:30-10:20 T11(J. Choi)
10:00			
		10:20-11:10 T5(Q. Xu)	10:20-11:10 T12(K. Okazaki)
11:00			
		11:10-12:00 T6(J. Liu)	11:10-12:00 T13(J. Lee)
12:00	**The time shown is Japan Standard Time.**	12:00-14:00 Lunch	
13:00			
14:00		14:00-14:50 T7(T. Tsuchimochi)	14:00-14:50 T14 (M. Hatanaka)
15:00	*15:00-15:10 Opening remarks*	14:50-15:40 T8(W. Mizukami)	14:50-15:40 T15(C. Shang)
	15:10-16:00 T1(L. Shen)	15:40-16:00 Coffee Break	*15:40- 16:00 Closing remarks*
16:00	16:00-16:50 T2(A. Mukaoka)	16:00-16:50 T9(J. Jiang)	
	16:50-17:40 T3(H. Shin)	16:50-17:40 T10(S. Choi)	
17:00			
18:00	17:40-19:30 Poster	17:40-19:30 Poster	
19:00			

Poster presentation

January 12 (Wednesday)

P1-01: **Baoshan Hou** (Shandong University)
Solution Environment and Electrode Interface: Theoretical Design of Corrosion Inhibitors in Complex Environment

P1-02: **Xiaoli Wang** (Shandong University)
Theoretical Calculation of Organic Host-Guest Doped Materials with Room Temperature Phosphorescence

P1-03: **Ning Zhang** (Peking University)
Iterative Configuration Interaction with Selection

P1-04: **Yitian Zhu** (Shandong University)
Density-based basis-set correction to iCIPT2

P1-05: **Ryo Fujisawa** (Waseda University)
Assessment and improvement of machine-learned electron correlation model based on applicability domain determination

P1-06: **Kento Kasahara** (Osaka University)
Elucidating the rate constant of host-guest binding based on molecular dynamics and diffusion-influenced reaction theory

P1-07: **Kyunghoon Lee** (KAIST)
A novel quantification method of drug-likeness based on unsupervised learning

P1-08: **Jong Hyeon Lim** (Sungkyunkwan University)
Computational research for therapeutic effect of photosensitizers through the excited state dynamics and band analysis

P1-09: **Suhwan Song** (Yonsei University)
BL1p: A Minimally Parameterized DC-DFT Functional

Poster presentation

January 13 (Thursday)

P2-01: **Yibo Lei** (Northwest University)
Imposed CASSCF (iCAS): Imposed Automatic Selection and Localization of Complete Active Spaces

P2-02: **Yangyang Song** (Shandong University)
Benchmarking SDSCI and SDSPT2

P2-03: **Linfeng Ye** (Shandong University)
Full Spectrum from Real-Time Time-Dependent Density Functional Theory with Large Time Step and Short Simulation Time

P2-04: **Taichi Inagaki** (Keio University)
Hamiltonian Monte Carlo Method with Potential Scaling for Canonical Multimodal Distributions and Relaxation Processes

P2-05: **Chinami Takashima** (Waseda University)
Acceleration of local unitary transformation method by utilizing database of atomic two-electron integrals

P2-06: **Hiroki Uratani** (Waseda University)
Nanoscale Excited-State Dynamics Simulations Using Semiempirical Quantum Chemical Calculations and Reduced-Scaling Approaches

P2-07: **Iulia Emilia Brumboiu** (Pohang University of Science and Technology)
Core-Excited State Analytical Gradients in the ADC framework

P2-08: **Woojin Park** (Kyungpook National University)
Relief of excited-state antiaromaticity enables the smallest red emitter

P2-09: **Seung-Jae Shin** (KAIST)
A mean-field QM/MM study revealing the aqueous electric double layer structure and its importance on the electrocatalysis