2020 International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry

Dec 04-07, 2020
Venue: Shenzhen, Guangdong, China

Program

Day1: December 04, 2020, Friday	
8:30-11:30	**Registration & Discussion**
11:30-13:45	**Lunch & Rest**
13:45-14:00	**Opening Remarks**
	Chairs: Hai-Qin Lin 林海青 (CSRC，北京计算科学研究中心) Zhi-Pan Liu 刘智攀 （FDU，复旦大学）
14:00-14:30	Feng-Long Gu 顾凤龙（SCNU，华南师范大学） 基于非正交定域分子轨道的线性标度方法
14:30-15:15	Wei-Tao Yang 杨伟涛（DUKE，美国杜克大学）（线上） Quantum Many-Electron Calculations at Mean-Field Costs: How Far Can Density Functional Theory Go?
15:15-15:35	Ying-Jin Ma 马英晋（CNIC, CAS，中科院计算机信息网络中心） Progress of low-scaling excited-state calculation by the virtue of AI@HPC
15:35-16:05	**Tea Break & Group Photo**
16:05-16:35	Xiang-Rong Wang 王向荣（HKUST，香港科技大学）(线上) Current-driving skyrmion motion in inhomogeneous films
16:35-17:05	Bing Huang 黄兵 (CSRC，北京计算科学研究中心) Developing Defect and Doping Theory in Semiconductors
17:05-17:25	Ji-Chang Ren 任吉昌 （NJUST，南京理工大学）（线上） Origin of unexpected large Seebeck effect in SrTiO3: nonperturbative polaron study from ab initio cumulant expansion
18:00-19:00	**Committee Meeting**

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Day2：December 05, Saturday，9:00 - 11:30 Discussion	
11:30-14:00	**Lunch & Rest**
14:00 – 17:00	
	Chairs: Fan-Qi Yuan 袁凡奇 (CSAR，深圳京鲁计算科学应用研究院) Ke-Li Han 韩克利 (DICP，CAS，中科院大连化物所)
14:00-14:30	Zhi-Pan Liu 刘智攀 （FDU，复旦大学） 从机器学习计算模拟到人工智能化学
14:30-15:00	Bing-Bing Suo 索兵兵 （NWU，西北大学） New development of Fock-like matrix algorithm in BDF
15:00-15:20	Hao-Jian Deng 邓皓键 （CSAR，深圳京鲁计算科学应用研究院） Low lying excitations in graphene: quantum Monte Carlo study
15:20-15:50	**Tea Break**
15:50-16:20	Wen-Jian Liu 刘文剑（SDU，山东大学） The Static-Dynamic-Static Framework for Strongly Correlated Electrons
16:20-16:40	Shu-Xian Hu 胡淑娴（USTB，北京科技大学） Band Gap Predictions of Semiconductors with Coupled Cluster Wavefunction-based Ab initio Methods
16:4-17:00	Cheng Shang 商城（FDU，复旦大学） Massively Parallelization Strategy for High-Dimensional Neural Network Potential
Banquet	

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Day3：December 06, Sunday， 9:00 - 11:30 Discussion	
11:30-14:00	**Lunch & Rest**
14:00 – 17:30	
	Chairs : Feng-Long Gu 顾凤龙 （SCNU，华南师范大学） John Z.H. Zhang 张增辉 （NYU Shanghai，上海纽约大学）
14:00-14:30	John Z.H. Zhang 张增辉 （NYU Shanghai，上海纽约大学） 蛋白相互作用与稳定性的理论计算
14:30-15:00	Xiao He 何晓 （ECNU，华东师范大学） Fragment Quantum Mechanical Methods: Beyond QM/MM and DFT
15:00-15:30	Tong Zhu 朱通（ECNU，华东师范大学） Force Field Development for Metalloproteins with Artificial Neural Networks
15:30-16:00	**Tea Break**
16:00-16:30	Wen-qing Zhang 张文清 （(SUSTech，南方科技大学） Thermoelectric Transports By Machine-learning Approach
16:30-17:00	Pei-Feng Su 苏培峰 (XMU，厦门大学) Energy decomposition analysis methods for complex systems
17:00-17:30	Zhen-Hua Chen 陈振华 (XMU，厦门大学) Electron transfer theory based on diabatic representation

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Day4：December 07, Monday, 9:00 - 11:30 Discussion	
11:30-14:00	**Lunch & Rest**
14:00 – 17:25	
	Chairs: Rui-Qin Zhang 张瑞勤 (CSRC，北京计算科学研究中心) Wen-Jian Liu 刘文剑 (SDU，山东大学)
14:00-14:45	Jia-Li Gao 高加力 （UMN，明尼苏达大学）(线上) Minimal active space for excited states through a dynamic-then-static approach
14:45-15:15	Ke-Li Han 韩克利 (DICP，CAS，中科院大连化物所) Charge carrier dynamics in perovskite nanocrystals
15:15-15:45	Wei Hu 胡伟（UCTC，中国科技大学） Introduction to HONPAS: Hefei Order-N Packages for Ab initio Simulations
15:45-16:15	**Tea Break**
16:15-16:35	Pavlo Dral（XMU，厦门大学） Making quantum chemistry more efficient with semiempirical and machine learning approaches
16:35-16:55	Yang Guo 郭阳 (SDU，山东大学) Linear-scaling explicitly correlated N-electron state valence perturbation theory with pair natural orbital (DLPNO-NEVPT2-F12)
16:55-17:25	Rui-Qin Zhang 张瑞勤 (CSRC，北京计算科学研究中心) Solutions of Schrödinger equations of atomic and molecular systems using a residual correction method