Programme Agenda

Time	Session	Chair
08:30	Welcome and introduction	
	Morning Session	
08:40	**Machine Learning Simulation using LASP: Current Status, New Development and Connection with Catalysis Experiment** Zhipan Liu, *Fudan University*	Nanfeng Zheng
09:20	**Applications of Machine-learning in Research and Development of Flow Batteries** Xianfeng Li, *Dalian Institute of Chemical Physics, CAS*	
09:45	**Computational Approach Towards New Porous Organic Cages Discovery** Shan Jiang, *ShanghaiTech University*	
09:55	**Machine Learning Assisted Catalysis Design for Electrochemical Reactions** Tao Cheng, *Soochow University*	
10:05	**The Rational Design of Catalysts Combining Machine Learning and Reaction Phase Diagram** Jianping Xiao, *Dalian Institute of Chemical Physics, CAS*	
10:15	Photo & Coffee Break	
10:40	**Deep Learning for Topology Optimization of Metamaterials** Liang Gao, *Huazhong University of Science and Technology*	Zhipan Liu
11:05	**Machine-Learning-Guided Discovery and Optimization of Additives in Preparing Cu Catalysts for CO_2 Reduction** Cheng Wang, *Xiamen University*	
11:15	**Atomly.net: Accelerating the Materials Science from Computation, Data and AI** Miao Liu, *Institute of Physics, CAS*	
11:25	**Accelerating Energy Materials Innovation from High-Throughput Computations and Screening to Artificial Intelligence** Zhen Zhou, *Nankai University/Zheng Zhou University*	
11:50	**Theoretical Investigation of Supported Cluster Catalysts** Jinxun Liu, *University of Science and Technology of China*	
12:00	**Royal Society of Chemistry – Supporting the Chemical Science Community in China** Hongmei Peng, *Royal Society of Chemistry*	
12:20	Lunch	

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Afternoon Session		
14:00	**Single-Molecule Fluorescence Imaging Analysis of Protein Stoichiometry via Deep Learning** Xiaohong Fang, *Institute of Chemistry, CAS*	Zhen Zhou
14:40	**Application of Deep Learning in Raman Spectroscopy and Imaging** Bin Ren, *Xiamen University*	
15:05	**The Development of LASP Software and Its Application in Heterogeneous Catalysis Simulation** Cheng Shang, *Fudan University*	
15:15	**Machine Learning Prediction of Magnetic Properties of Fe-based Metallic Glasses with Applications of Energy-Saving Technology** Guangcun Shan, *Beihang University*	
15:40	**Understanding the Structures and Photocatalytic Properties of Carbon Nitride from a Molecular Level** Wei Lin, *Fuzhou University*	
15:50	**Electrochemical NMR: A Powerful Tool in Electrocatalysis Study** Shuohui Cao, *Xiamen University*	
16:00	Coffee Break	
16:20	**Simple Descriptor Derived from Symbolic Regression Accelerating the Discovery of New Perovskite Catalysts** Wanjian Yin, *Soochow University*	Xiaohong Fang
16:45	**Molecular-level Design of Nanoreactors towards Next Generation Electrode Materials** Jian Liu, *Dalian Institute of Chemical Physics, CAS*	
16:55	**Prediction of Reactivity and Selectivity in Organic Synthesis via Machine Learning** Xin Hong, *Zhejiang University*	
17:20	**Hierarchical High-Throughput Screening and Machine Learning Algorithm Accelerate the Discovery of Efficient Electrocatalysts for Ammonia Synthesis** Liming Yang, *Huazhong University of Science and Technology*	
17:30	**Predict the Stability and Catalytic Performance of Nitrogen-doped Carbon Nanocones by Machine Learning** Guoliang Chai, *Fujian Institute of Research on the Structure of Matter, CAS*	
17:55	**ReaxFF Force Field Development and Application in Supercritical Water Reaction** You Han, *Tianjin University*	
18:05	Closing	