

ICT-HPCC22 Schedule									
	Jul 12th Tuesday				Jul 13th Wednesday				
Morning Session	Session Chair	Beijing Time	Title	Speaker	Session Chair	Beijing Time	Title	Speaker	
	No Report				TBD	10:00 - 10:30	Studying strongly correlated materials with density matrix embedding theory (DMET)	Chong Sun	
						10:30 - 11:10	High-performance supercomputing-powered design, discovery and development of first-in-class therapeutics: A journey from in silico to clinical studies	Chang-Guo Zhan	
						11:10 - 11:20	Break		
					Masaaki Saitow	11:20 - 11:40		Quan Phung	
						11:40 - 12:10	Fast evaluation of exchange in periodic systems	Sandeep Sharma	
Noon Break									
Afternoon Session	Session Chair	Beijing Time	Title	Speaker	Session Chair	Beijing Time	Title	Speaker	
	Zhong Jin	14:00 - 14:40	Opening Conference		Lixin He	14:00 - 14:20	Block2: A versatile tool for modern ab initio DMRG	Huanchen Zhai	
		14:40 - 15:10	Exact two-component Hamiltonians for scalable relativistic quantum chemistry	Stefan Knecht		14:25 - 14:55	TBD	Honghui Shang	
						14:55 - 15:15	TBD	Haicang Zhang	
		15:10 - 15:25	Break			15:15 - 15:30	Break		
	Stefan Knecht	15:25 - 15:55	De novo protein design with neural network energy functions learned from data	Haiyan Liu	Zhendong Li	15:30 - 16:00	Efficient implementation of hybrid functionals in ABACUS, a first-principles package based on atomic orbital bases	Lixin He	
		15:55 - 16:25	G Protein-Coupled Receptors: from Structure to Mechanism	Qingtong Zhou		16:00 - 16:30	Stochastic adaptive single-site algorithm and hierarchical mapping for TD-DMRG	Haibo MA	
	Late Break								
Evening Session	Session Chair	Beijing Time	Title	Speaker	Session Chair	Beijing Time	Title	Speaker	
	Alberto Baiardi	18:30 - 19:00	TBD	Masaaki Saitow	TBD	18:30 - 19:00	Time-dependent DMRG for molecular quantum dynamics with anharmonic potentials	Jiajun Ren	
		19:00 - 19:35	Excited-state machine learning molecular dynamics	Philipp Marquetand		19:00 - 19:30	Investigating quantum many-body problems with quantum processors	Chen Cheng	
		19:35 - 19:45	Break			19:30 - 19:40	Break		
	Haibo MA	19:45 - 20:15	New Density Matrix Renormalization Group-based Methods for Molecular Simulations	Alberto Baiardi	TBD	19:40 - 20:05	TBD	Yue Kong	
		20:15 - 20:45	Ab initio Comb Tensor Network States for Polynuclear Transition Metal Complexes	Zhendong Li		Jin Zhong	20:05 - 20:35	Development of free energy perturbation based drug discovery methods and their applications	Zhe Li
					Closing Conference				