Program

Oct. 26 (Wed)

13:00-13:10	Opening		Kazuo Akagi (Director), Shigeyoshi Sakaki
		Chair	Shigeyoshi Sakaki (Kyoto)
13:10-13:45	PL1	Feliu Maseras (Tarragona)	Single electron transfer processes in homogeneous catalysis
13:45-14:00	Break		
		Chair	Mitsutaka Okumura (Osaka)
14:00-14:25	1-1	Romuald Poteau (Toulouse)	Ruthenium nanoclusters in equilibrium with syngas: a DFT study
14:25-14:50	1-2	Hiromi Nakai (Tokyo)	Divide-and-conquer density-functional tight-binding molecular-dynamics (DC-DFTB-MD) simulations for nano-scale chemical reaction systems
14:50-15:15	1-3	Nuria Lopez (Tarragona)	Single Site Chemistry: Converging strategies in catalysis
15:15-15:40	1-4	Takashi Kamachi (Fukuoka)	Low-Mode Conformational Search Method with Semi-empirical Quantum Mechanical Calculations: Application to Enantioselective Organocatalysis
15:40-16:00	Break		
		Chair	Miho Hatanaka (Osaka)
16:00-16:25	1-5	Yuki Kurashige (Kobe)	Strong-correlation in catalytic center of biological and artificial systems
16:25-16:50	1-6	Agusti Lledos (Barcelona)	Organometallic enzyme hybrid catalysts: computational challenges
16:50-17:15	1-7	Shusuke Yamanaka (Osaka)	Development of a new computational method to design of catalytic fields
17:15-17:40	1-8	Lionel Perrin (Lyon)	Computational inputs for industrial applications in polymerization catalysis
17:40-17:50	Break		
		Chair	Shigeru Nagase (Kyoto)
17:50-18:25	PL2	Odile Eisenstein (Montpellier)	Understanding NMR chemical shifts: an old problem and new results
18:30-19:00		Poster Short talk	(3 min/one person)
19:00-20:30	Poster Session		

Oct. 27 (Thu)

		Chair	Masataka Nagaoka (Nagoya)
9:30-9:55	2-1	Mikiya Fujii (Tokyo)	Computational description of charge dissociation in organic photovoltaics
9:55-10:20	2-2	Alessandro Genoni (Nancy)	Recent Advances in the Determination of “Experimental” Wave Functions
10:20-10:45	2-3	Tetsuya Taketsugu (Sapporo)	On-the-fly dynamics study on the photoisomerization mechanism of stilbene and its derivative
10:45-11:00	Break		
		Chair	Masataka Nagaoka (Nagoya)
11:05-11:30	2-4	Nicolas Ferre (Marseille)	Modulation of Anabanena Sensory Rhodopsin photophysical properties with pH: insights from QM/MM and MD calculations
11:30-11:55	2-5	Shigehiko Hayashi (Kyoto)	Crucial role of protein flexibility in enzymatic catalysis
11:55-12:20	2-6	Vicent Moliner (Castelló de la Plana)	Computer assisted design of new biocatalyst
12:20-13:50	Lunch		
		Chair	Kazunari Yoshizawa (Fukuoka)
13:50-14:15	2-7	Gonzalo Jimenez-Oses (La Rioja)	Tuning the Structure and Dynamics of Flexible Regions in Engineered Enzymes
14:15-14:40	2-8	Sonsoles Martin-Santamaria (Madrid)	Innate immunity Toll-like receptors. Computational approaches to their molecular recognition events
14:40-15:05	2-9	Shoji Takada (Kyoto)	Multiscale computational modeling for giant biomolecular complexes
15:05-15:30	2-10	Laura Masgrau (Barcelona)	Computational modeling of enzyme-catalyzed reactions
15:30-15:45	Break		

		Chair	Kazunari Yoshizawa (Fukuoka)
15:50-16:15	2-11	Carine Michel (Lyon)	When modeling bridges electrocatalysis and heterogeneous catalysis: the case of the formic acid decomposition (Temporary)
16:15-16:40	2-12	Akira Nakayama (Sapporo)	Catalytic reactions at the liquid/metal-oxide interface: role of the acid-base sites
16:40-17:05	2-13	Eric Clot (Montpellier)	DFT Studies of copper-catalyzed formation of amide from alcohol and amine
17:05-17:20		Break	
		Chair	Koichi Yamashita (Tokyo)
17:20-17:55	PL3	Hiroshi Nakatsuji (Kyoto)	Chemistry of the excited states studied by the SAC-CI theoretical methodology
18:15-20:15	Banquet	Fukui Center	

Oct. 28 (Fri)

		Chair	Jyun-ya Hasegawa (Sapporo)
9:30-9:55	3-1	Ryoichi Fukuda (Kyoto)	Modeling molecular systems at extreme pressure: confined electronic excited states, photochemistry, and circular dichroism
9:55-10:20	3-2	Marcel Swart (Girona)	Spinning around in transition-metal chemistry
10:20-10:45	3-3	Minori Abe (Tokyo)	Search of electric dipole moment of an electron as a probe of CP violation: Role of theoretical chemistry
10:45-11:00	Break		
		Chair	Jyun-ya Hasegawa (Sapporo)
11:00-11:25	3-4	Shinji Tsuneyuki (Tokyo)	First-principles calculation and modeling of thermal transport in heavily anharmonic crystals
11:25-11:50	3-5	Julia Contreras-Garcia (Paris)	Quantum topology: Understanding new chemistries with old concepts
11:50-12:15	3-6	Kazuo Takatsuka (Kyoto)	Quantum Chemistry beyond the Born-Oppenheimer Approximation
12:15-13:45		Lunch	
		Chair	Masahiro Ehara (Okazaki)
13:45-14:10	3-7	Masayoshi Nakano (Osaka)	Quantum Design for Optoelectric Functional Molecular Systems
14:10-14:35	3-9	Fernando Cossio (Vizkaya)	Emergent properties in nonbonding and bonding interactions
14:35-15:00	3-10	Manuel Ruiz-Lopez (Nancy)	Solvation effects at the air-water interface on the near-UV photolysis of tropospheric oxidants
15:00-15:25	3-11	Hirofumi Sato (Kyoto)	Chemical processes in condensed phase: Quantum chemistry and statistical mechanics
15:25-15:35	Closing	Odile Eisenstein (Montpellier)	