

ICCC2018 Program (S28)

July 30, 2018 (Mon)		July 31, 2018 (Tue)		Aug 1, 2018 (Wen)		Aug 2, 2018 (Thu)		Aug 3, 2018 (Fri)		Aug 4, 2018 (Sat)	
		8:30	Plenary Lecture	8:30	Plenary Lecture	8:30	Plenary Lecture	8:30	Plenary Lecture <b>Prof. Shie-Ming Peng</b>	8:30	Plenary Lecture
		9:15		9:15		9:15		9:15	Coffee Break	9:15	
		9:40		9:40		9:40		9:40	Laura Gagliardi	9:40	
		10:05		10:05		10:05		10:05	Heather Kulik	10:05	
		10:25		10:25		10:25		10:25	Jermy Harvey	10:25	
		10:45		10:45		10:45		10:45	Liviu Ungur	10:45	
		11:00		11:00		11:00		11:00	Jean-Francois Halet	11:00	
		11:15		11:15		11:15		11:15	Alessandro Lunghi	11:15	
		11:30		11:30		11:30		11:30	Elizaveta Suturina	11:30	
		11:45		11:45		11:45		11:45	Jun Zhu	11:45	
		12:00		12:00		12:00		12:00	Kechen Wu	12:10	<b>Special Lecture:Prof. Jean-Pierre Sauvage</b>
		12:15		12:15		12:15		12:15	Lunch		
		13:15	Plenary Lecture	13:15	Plenary Lecture		13:15	Plenary Lecture <b>Prof. James Mayer</b>	13:10		
		14:00		14:00			14:00	Coffee Break			
		14:25		14:25			14:25	Stefan Grimme			
14:50		14:50		14:50	Dimitrios Pantazis						
15:10		15:10		15:10	Nuria Lopez						
15:30		15:30		15:30	Maylis ORIO						
15:50		15:50		15:50	Steven Roldan-Gomez						
16:05		16:05		16:05	Panida Surawatanawong						
16:20		16:20		16:20	Coffee Break						
16:45		16:45		16:45	Kazunari Yoshizawa						
17:10		17:10		17:10	Miho Hatanaka						
17:30		17:30		17:30	Mitsuo Shoji						
17:50		17:50		17:50	Sameera W. M. C.						
18:00	<b>Special Lecture: Prof. Eiichi Negishi</b>	18:05		18:05			18:45	Banquet @ Hotel Metropolitan Sendai			
18:20		18:20		18:20							
19:00		18:35		18:35		18:30	<b>Poster Session of S28 (this session)</b>				
						20:30					

Session	Lecture	Poster Date	Code	Name	Affiliation	Title
S28	Organizer			Eliseo Ruiz	Universitat de Barcelona	
S28				Laura Gagliardi	University of Minnesota	
S28				Daniel Aravena	University of Santiago de Chile	
S28				Gopalan Rajaraman	Indian Institute of Technology Bombay	
S28				Yu Takano	Hiroshima City University	
S28				Yasutaka Kitagawa	Osaka University	
S28	Keynote		A00247-LG	Laura Gagliardi	University of Minnesota	Modeling metal-containing systems with multireference methods
S28	Keynote		A00344-SG	Stefan Grimme	University of Bonn, Mulliken Center for Theoretical Chemistry	Recent Progress with Low-Cost Quantum Chemistry
S28	Keynote		A01438-KY	Kazunari Yoshizawa	Kyushu University	Quantum chemical studies on catalytic and enzymatic reactions mediated by transition-metal complexes
S28	Invited		A00725-HK	Heather Kulik	Massachusetts Institute of Technology	Overcoming functional sensitivity in DFT predictions of spin state ordering
S28	Invited		A03043-JH	Jermy Harvey	Department of Chemistry, KU Leuven	Spin-Forbidden Oxidation Chemistry of Metal-Oxo Species: Insights from Ab Initio and DFT
S28	Invited		A01341-DP	Dimitrios Pantazis	Max Planck Institute for Coal Research	Theoretical perspectives on biological water oxidation: electronic structure determinants of catalytic control
S28	Invited		A01931-NL	Nuria Lopez	Institute of Chemical Research of Catalonia, The Barcelona Institute of Science and Technology	Single Atom Catalysis: the missing link between Homogeneous and Heterogeneous Catalysis
S28	Invited		A00343-MO	Maylis Orio	CNRS-AMU	Experimental and theoretical studies of the electrocatalytic hydrogen production by thiosemicarbazone metal complexes
S28	Invited		A02037-MH	Miho Hatanaka	Nara Institute for Science and Technology	Computational study on the lanthanide luminescent materials
S28	Invited		A00169-MS	Mitsuo Shoji	Center for Computational Sciences, University of Tsukuba	QM/MM study on the S state transitions of the Oxygen Evolving Complex in Photosystem II
S28	Oral Talk		A01389-LU	Liviu Ungur	National University of Singapore	Ab Initio Crystal Field for Lanthanides
S28	Oral Talk		A00413-JH	Jean-Francois Halet	Institut des Sciences Chimiques de Rennes, CNRS-Universite de Rennes	On the Search of Novel Molecules Demonstrating Quantum Cellular Automata Properties. A Theoretical Approach
S28	Oral Talk		A01277-AL	Alessandro Lunghi	Trinity College Dublin	First Principle determination of Spins and Phonons Relaxation mechanisms in Molecular Magnets
S28	Oral Talk		A00829-JZ	Jun Zhu	Department of Chemistry, Xiamen University	Adaptive Aromaticity: 16-Electron Osmapentalene Being Aromatic in both the S0 and T1 states
S28	Oral Talk		A00905-KW	Kechen Wu	Chinese Academy of Sciences	Second-order nonlinear optical properties of transition-metal cluster compounds
S28	Oral Talk		A01185-SR	Steven Roldan Gomez	Universitat de Girona	Shedding light into the mechanism of a cobalt-catalyzed C-H functionalization with diazo esters by computational means. The case of the aryl-Co(III) masked-carbene intermediates
S28	Oral Talk		A01611-PS	Panida Surawatanawong	Department of Chemistry, Faculty of Science, Mahidol University	Mechanisms of C-O and H2 Activation: Density Functional Study

S28	Oral Talk		A01941-SW	Sameera W. M. C.	Hokkaido University	On the mechanism and selectivity of Fe-catalyzed carbon-carbon bond formation reactions
S28	Oral Talk		A02042-ES	Elizaveta Suturina	University of Southampton	Ligand field design for MRI contrast agents
S28	Poster	August 2	S28-P01	Toru Saito	Hiroshima City University	Transition State Search Using rPM6 Method: Applications to Oxidation Reactions Catalyzed by Transition Metal Complexes
S28	Poster	August 2	S28-P02	Dandan Chen	Department of Chemistry, Xiamen University	Reaction Mechanism of Iron(III) Catalyzed Carbonyl-Olefin Metathesis: A Computational Study
S28	Poster	August 2	S28-P03	Qin Zhu	Xiamen University	[3+2] Cycloaddition Reactions of Azides with Metal-carbyne Complexes: A Theoretical Study
S28	Poster	August 2	S28-P04	Yu Takano	Graduate School of Information Sciences, Hiroshima City University	Statistical and quantum-chemical analysis of the effect of heme porphyrin distortion in heme proteins
S28	Poster	August 2	S28-P05	Yuki Tsutsumi	Department of Advanced Materials Science, Faculty of Engineering, Kagawa University	Change of the electronic structure of tetra-coordinated metal complex by molecular distortion
S28	Poster	August 2	S28-P06	Daniel Aravena	Universidad de Santiago de Chile	Tuning spectroscopic and chemical properties of CuN4 complexes: a combined experimental and computational study
S28	Poster	August 2	S28-P07	Iori Era	Osaka University	Theoretical study of the relationship between ionization potentials and hydrogen bonds in 2Fe-S ferredoxin
S28	Poster	August 2	S28-P08	Hayato Tada	Osaka University	Theoretical study on single-molecular electron conductivity of paddlewheel-type acetate-bridged binuclear complexes
S28	Poster	August 2	S28-P09	Shogo Aoki	Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University	Theoretical study of metal ion effect on electronic structures and optical properties of bis(dipyrrinato) complexes
S28	Poster	August 2	S28-P10	Po-Jung Huang	Institute for Materials Research, Tohoku University	Experimental and Theoretical Studies on Frontier Orbitals of Carboxylate-bridged dichromium(II,II) complexes
S28	Poster	August 2	S28-P11	Masaya Yamasaki	Department of Advanced Materials Science, Faculty of Engineering, Kagawa University	Prediction of superatom by molecular orbital method
S28	Poster	August 2	S28-P12	Koki Soeda	University of Tsukuba	Analysis of metal-metal bonds in Ag(I) ions complexes by density functional theory
S28	Poster	August 2	S28-P13	Muzzaffar Bhat	Islamic University of Science and Technology	1-(chlorophenyl)-4-(3-phenylseleno propyl) piperazine (L1); Synthesis, spectroscopic characterization, DFT studies, biological activity and its reactivity towards group 12 metal chlorides.
S28	Poster	August 2	S28-P14	Koichi Miyagawa	Osaka University	UNO-DMRG calculations of effective exchange integrals for binuclear manganese complexes
S28	Poster	August 2	S28-P15	Takeyoshi Oguma	Department of Advanced Materials Science, Faculty of Engineering, Kagawa University, Japan	Controlling of the spin crossover by Jahn-Teller distortion in octahedral hexa-coordinate complex.