

International Symposium "Theoretical Design of Materials with Innovative Functions Based on Element Strategy and Relativistic Electronic Theory"

Place: International House of Tokyo Metropolitan University
Date: 8-9, December 2017

Friday (8 December 2017) Room 1			
Chairperson: Masahiko Hada			
A1	10:00-10:20	Hiromi Nakai (Waseda Univ., Japan)	Opening Address
A2	10:20-11:00	Trond Saue (Univ. Toulouse, France)	Beyond the Electric Dipole Approximation in Relativistic Simulations of X-ray Spectroscopy
11:00-11:30		Coffee Break	
Chairperson: Takahito Nakajima			
A3	11:30-12:10	Jun Li (Tsinghua Univ., China)	Relativity-Induced Chemical Bonding Picture Change in Heavy-Element Compounds
A4	12:10-12:30	Junji Seino (Waseda Univ., Japan)	RAQET: Large-Scale Two-Component Relativistic Quantum Chemistry Program Package
12:30-14:00		Lunch	
Chairperson: Trond Saue			
A5	14:00-14:40	Maria Barysz (Nicolaus Copernicus Univ., Poland)	Electronic Structure of Gold Clusters: SiAu, SiAu ⁺ and SiAu ⁻
A6	14:40-15:20	Roland Lindh (Uppsala Univ., Sweden)	Non-Adiabatic Chemiluminescent Dynamics of the Methyl-Substituted 1,2-Dioxetanes
A7	15:20-15:40	Takao Tsuneda (Univ. of Yamashina, Japan)	Role of Metal ion Hydration Complexes in H ₂ O ₂ Decomposition Reactions
A8	15:40-16:00	Yukiomi Kita (Yokohama City Univ., Japan)	First-Principles Study on the Binding of a Positron to Polyatomic Molecules
16:00-16:30		Coffee Break	
Chairperson: Yutaka Imamura			
A9	16:30-17:10	Christel M. Marian (Heinrich-Heine-Univ., Germany)	Intersystem Crossing in Coinage-Metal Coordination Complexes and Metal-Free TADF Emitters
A10	17:10-18:00	Vladimir G. Malkin & Olga L. Malkina (Slovak Academy Science, Slovakia)	Calculations of the EPR Parameters Using Unrestricted Two- and Four-Component Relativistic Approaches within the HF and DFT Frameworks
A11	18:00-18:20	Jun-ya Hasegawa (Hokkaido Univ., Japan)	Constraint Structure Optimization for Minimum Energy Intersystem Crossing Point
Move to Restaurant			
18:30-20:30		Banquet	
Saturday (9 December 2017) Room 1			
Chairperson: Jun-ya Hasegawa			
B1	8:40-9:20	Lucas Visscher (Vrije Uni. Amsterdam, The Netherlands)	Obtaining Transition Moments in Relativistic Correlated Calculations
B2	9:20-10:00	Kenneth G. Dyall (Schrodinger Inc., USA)	Efficient Use of Basis Sets in Relativistic Calculations for Materials
10:00-10:30		Coffee Break	
B3	10:30-11:10	Markus Reiher (ETH Zurich, Switzerland)	From Relativistic DMRG Calculations to the Exploration and Automated Benchmarking of Functional Chemical Networks
B4	11:10-11:50	Jürgen Gauss (Gutenberg-Univ. Mainz, Germany)	Spin-Free Relativistic Quantum Chemistry: Analytic Gradients and Spin-Orbit Corrections
B5	11:50-12:10	Nobuki Inoue (AIST, Japan)	Study on Negative Kinetic Energy Spinors in Relativistic Electron Correlation Theory
B6	12:10-12:30	Satoshi Yabushita (Keio Univ., Japan)	Hypersensitive Transitions and Metal-Ligand Interactions in Lanthanide Complexes
12:30-12:45		Assembly Photo	
12:45-14:00		Lunch	
Chairperson: Minori Abe			
B7	14:00-14:40	Kenneth Ruud (Univ. of Tromsø)	4-Component Relativistic Calculations with Periodic Boundary Conditions
B8	14:40-15:00	Yutaka Imamura (Tokyo Metropolitan Univ., Japan)	Theoretical Study on Spin-Forbidden Transition for Dye-Sensitized Solar Cell
P	15:00-16:30	Poster Sesseion at Lobby	
Chairperson: Vladimir Malkin			
B9	16:30-17:10	Bijaya K. Sahoo (Physical Research Laboratory, India)	Relativistic Normal Coupled-cluster Theory of Atomic Electric Dipole Moments
B10	17:10-17:30	Minori Abe (Tokyo Metropolitan Univ., Japan)	Relativistic calculations of parity and time reversal violation effects in atoms and molecules
17:30-17:40		Closing Remarks	