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
Poster Presentation

	Name	Affllliation	Title
1	Michiko Atsumi	University of Oslo	^{13}C Nuclear Magnetic Shielding Constants for Excited States
2	Renu Bala	Indian Institute of Technology Roorkee	Calculations of Magnetic Hyperfine Structure Constants for Alkaline-Earth Monofluorides
3	Mikito Fujinami	Waseda University	Chemical Reaction Prediction and Analysis Based on Informatics with Quantum Chemical Descriptors
4	Kenta Hiraga	Waseda University	Development of Spin-Dependent Relativistic Time-Dependent Density Functional Theory Based on Infinite-Order Douglas-Kroll-Hess Method
5	Takahiro Hirai	Waseda University	Theoretical Study of Temperature and Pressure Dependences of NO-CO Reactions on Rh(111) Surface
6	Yasuhiro Ikabata	Waseda University	Time-Dependent Density Functional Study on Near-Infrared Absorption of Trioxotriangulene Derivatives
7	Minori Imai	Waseda University	Theoretical Research of Primary Proton Transfer in Bacteriorhodopsin Using DC-DFTB-Metadynamics
8	Ryo Kageyama	Waseda University	Semi-Local Machine Learned Kinetic Energy Functional for Orbital-Free DFT
9	Muneaki Kamiya	Gifu University	Development of Two-Component Relativistic Time-Dependent Density Functional Theory and its Analytical Gradient
10	Shohei Kanno	Tokyo Metropolitan University	Theoretical Study on Rotational Controllability of Organic Cations in Hybrid Perovskites
11	Masato Kobayashi	Hokkaido University	All-Electron Relativistic Computations on the Low-Lying Electronic States of CeF with Spin-Orbit Coupling Effects
12	Nawee Kungwan	Chiang Mai University	Solvent Dependence of Double Proton Transfer in the Formic Acid -Formamidine Complex: Path Integral Molecular Dynamics Investigation
13	Masaya Miyamoto	Tokyo Metropolitan University	Analysis of HALA effects in Relativistic NMR Calculation Using Singular Value Decomposition
14	Reo Murata	Tokyo Metropolitan University	Theoretical Study on Halogen-Passivated Quantum Dot Solar Cell
15	Naoki Nakatani	Tokyo Metropolitan University	Density Matrix Renormalization Group in Practice: Applications to Strongly Correlated Molecular Systems
16	Yoshifumi Nishimura	Waseda University	DC-DFTB-K: A Massively Parallel Chemical Reaction Dynamics Simulator for Huge Systems
17	Junichi Ono	Waseda University	Proton Delocalization in Proton Releasing Group of Bacteriorhodopsin Using DC-DFTB-MD Simulations
18	Yusuke Ootani	Tohoku University	First-Principles Molecular Dynamics Study on Chemical Reaction of Silicon-Based Materials Induced by Friction
19	Takuro Oyama	Waseda University	Two-Component Relativistic Density Functional Theory with Picture-Change Corrected Electron Density
20	Nattapong Paiboonvorachat	Chulalongkorn University	DFT Investigation on the Orientation of CoPc Molecules in Thin Film on Co Substrate
21	Manabu Sugimoto	Kumamoto University	Evaluation of Electronic 3D Shape Similarity and Its Applications
22	Ayaki Sunaga	Tokyo Metropolitan University	Analysis of Effective Electric Fields of Heavy Molecules for Electron Electric-Dipole-Moment Searches
23	Kazuo Toyota	Osaka City University	Formulation of Coupling Anisotropy Function for Symmetry-Adapted-Cluster Configuration-Interaction Theory
24	Takashi Tsutsui	Tokyo Metropolitan University	P and T Symmetry Violation in Diamagnetic Molecules: Schiff Moment Calculations at Relativistic CCSD Level
25	Xiao-Gen Xiong	Institute for Molecular Science	Probing Chemical Bonding and Electronic Structures of ThO_n^- (n = 1, 2, 3) by Photoelectron Spectroscopy and Quantum Chemical Calculations
26	Jun Yi	Tokyo Metropolitan University	Vanadium NMR Chemical Shifts of (Imido)Vanadium(V) Dichloride Complexes: A Cooperation with QC Calculations and MLR Analyses
27	Takeshi Yoshikawa	Waseda University	Computerized Implementation of Divide-and-Conquer-Based Higher-Order Electron-Correlation Methods
28	Terutaka Yoshizawa	Tokyo Metropolitan University	Calculations of Nuclear Magnetic Shielding Constants Based on the Two-Component Normalized Elimination of the Small Component Method
29	Liming Zhao	Hokkaido University	Theoretical Study on Rh-Catalyzed Hydrosilylation of C=C and C=O Double Bonds