No.	Author(s)	Affiliation(s)	Title
1	**Kenichi Koizumi, Katsuyuki Nobusada, Mauro Boero**	Institute of Molecular science, Japan, ESICB, Kyoto University, Japan, IPCMS, France	**Simple but efficient method for inhibiting sintering of catalytic Pt nano-clusters on metal-oxide support evidenced by Car-Parrinello Molecular Dynamics Simulation**
2	**Sagarmoy Mandal, Jayashrita Debnath, Nisanth N Nair**	Department of Chemistry, Indian Institute of Technology Kanpur, India	**Ab Initio MD Simulations with Hybrid Functionals: Implementation and Application**
3	**Tatsuhiko Ohto**	Graduate School of Engineering Science, Osaka University, Japan	**Trimethylamine-N-oxide: its hydration structure and surface activity, viewed by vibrational spectroscopy and molecular dynamics simulations**
4	**Sushma Yadav, Amalendu Chandra**	Department of Chemistry, Indian Institute of Technology Kanpur, India	**Anisotropic Solvation Structure, Polarity and Dynamics of Polyoxyanions in Aqueous Solutions from Car-Parrinello Molecular Dynamics Simulations**
5	**K. Soniya, S. Awasthi, N.N. Nair and A. Chandra**	Department of Chemistry, Indian Institute of Technology Kanpur, India	**Mechanism and Free Energy Pathways of Transimination Reaction at the Active Site of Aspartate Aminotransferase (AspAT) in Aqueous Medium**
6	**Danjo De Chavez, Jun-ya Hasegawa**	Graduate School of Chemical Sciences and Engineering, Hokkaido University, Japan	**Directional Dependence of Ea Changes in Mechanochemical Activation**
7	**H. Sawada, K. Kawakami, F. Kormann, B. Grabowski, T. Hickel, J. Neugebauer**	Nippon Steel & Sumitomo Metal Corporation, Japan, Max-Planck-Institut für Eisenforschun, GmbH, Germany	**Partitioning of Cr and Si between cementite and ferrite derived from first-principles thermodynamics**
8	**Akira Nakayama, Masazumi Tamura, Ken-ichi Shimizu, Jun-ya Hasegawa**	Institute for Catalysis, Hokkaido University, Japan, JST PRESTO, Japan, Graduate School of Engineering, Tohoku University, Japan	**Catalytic Reactions at the Water/CeO2 Interface: Hydration of 2-Cyanopyridine**
9	**Hiroshi Nakano, Hirofumi Sato**	Graduate School of Engineering & Elements Strategy Initiative for Catalysts and Batteries, Kyoto University, Japan	**A Variational and perturbative approach to calculate nonequilibrium free energies for studying electron transfer reactions**
10	**Naoki Tsunoda, Yu Kumagai, Fumiyasu Oba**	Institute of Innovative Research & MCES, Tokyo Institute of Technology, Japan	**Ab Initio Study of Point Defects and p-Type Doping in ScN**
11	**Toshikazu Fujimori, Masato Kobayashi, Tetsuya Taketsugu**	Graduate School of Chemical Sciences and Engineering, Hokkaido University, Japan, JST PRESTO, Japan, Elements Strategy Initiative for Catalysts and Batteries, Kyoto University, Japan	**Automatic error control in the divide and conquer quantum chemical calculations**
12	**M. Shishkin, H. Sato**	Element Strategy Initiative for Catalysts and Batteries (ESICB) & Department of Molecular Engineering, Kyoto University, Japan	**Analysis of redox and magnetic properties of transition metal compounds using DFT+U with magnetic exchange method**
13	**Sho Imoto, Dominik Marx**	Lehrstuhl für Theoretische Chemie, Ruhr-Universtät Bochum, Germany	**Theoretical Vibrational Spectroscopy of Aqueous TMAO Solution under High Hydrostatic Pressure Conditions**
14	**Hiroki Uratani, Koichi Yamashita**	Department of Chemical System Engineering, School of Engineering, The University of Tokyo, Japan, JST CREST, Japan	**Inorganic Lattice Fluctuation Induces Charge Separation in Lead Iodide Perovskites: Theoretical Insights**
15	**Koichiro Kato, Masahiko Machida, Motoyuki Shiga**	Mizuho Information and Research Institute Inc., Japan, CCSE, Japan Atomic Energy Agency, Japan	**Nuclear quantum effects of light and heavy water studied by all-electron first principles path integral simulations**
16	**Yasuhide Mochizuki, Hirofumi Akamatsu, Yu Kumagai, Fumiyasu Oba**	Institute of Innovative Research & Materials Research Center for Element Strategy, Tokyo Institute of Technology, Japan	**Peierls Instability of a Layered Perovskite La3Ni2O7 under Biaxial Compressive Strain via First-Principles Calculations**
17	**Maofeng Dou, Shota Iizuka,Yasuaki Einaga, Yoshitaka Tateyama**	Center for Green Research on Energy and Environmental Materials, National Institute of Materials Science (NIMS), Japan, JST-ACCEL, Japan, Department of Chemistry, Keio University, Japan	**Termination effects on CO2 Reduction at Boron-doped Diamond electrodes: An Ab-initio Study**
18	**Shun Kikuchi, Shin Kiyohara, Teruyasu Mizoguchi**	Institute of Industrial Science, The University of Tokyo, Japan	**Making "Universal"-predictor to achieve high-throughput structure determination of oxcide grain boundaries**
19	**Lucie Szabova, Matteo Farnesi Camellone, Fabio Negreiros Ribeiro, Yoshitaka Tateyama, Stefano Fabris**	Center for Green Research on Energy and Environmental Materials, National Institute for Materials Science (NIMS), Japan, CNR-IOM DEMOCRITOS & SISSA, Italy	**Molecular dynamics simulation of water dynamics at the water/solidinterface of ceria-supported Pt clusters**

20	**Taedaehyung Eom, Hyungjun Kim, Ki-Ha Hong**	Graduate School of EEWS, Korea Advanced Institute of Science and Technology, Korea, Department of Materials Science and Engineering, Hanbat National University, Korea	**Understanding the Phase Stabilization Induced by Compositional Engineering of Organic-Inorganic Hybrid Perovskites**
21	**Miso Lee, Doyeon Kim, Kanghoon Yim, Seungwu Han**	Department of Materials Science and Engineering, Seoul National University, Korea, Korean Institute of Energy Research, Korea	**Non-oxide High-k Materials Screened by Automated Ab Initio Calculations**
22	**Masato Takenaka, Takeshi Iwasa, Tetsuya Taketsugu2**	Graduate School of Chemical Sciences and Engineering, Hokkaido University, Japan	**Theoretical Study on Near-field Infrared Absorption Spectroscopy using the Multipolar Hamiltonian**
23	**Shota Iizuka, Yoshitaka Tateyama**	Center for Green Research on Energy and Environmental Materials (GREEN), National Institute for Materials Science (NIMS), Japan	**DFT-D3 implementation in CPMD program for investigation of organic electrolyte solution**
24	**M. H. N. Assadi, Y. Tateyama**	Center for Green Research on Energy and Environmental Materials, National Institute for Materials Science (NIMS), Japan, Center for Computational Sciences, University of Tsukuba, Japan.	**Oxygen Contribution to Redox in Ilmenite Type 4d Transition Metal Oxides; Applications in Na ion Batteries**
25	**Makito Takagi, Satoshi Maeda**	Graduate School of Chemical Sciences and Engineering, Hokkaido University, Japan	**Exhaustive search for carbon crystal structures by artificial force induced reaction method**
26	**Yoritaka Furukawa, Yu-ichiro Matsushita**	The University of Tokyo, Japan	**Determining the densities of amorphous materials from first-principles calculations**
27	**Kyuhyun Lee, Wonseok Jeong, Dongheon Lee, Seungwu Han**	Department of Materials Science and Engineering Seoul National University, Korea	**Development of neural network interatomic potential and improve its reliability using training data analysis**
28	**Randy Jalem, Masanobu Nakayama**	JST-PRESTO, Japan, Global Research Center for Environment and Energy based on Nanomaterials Science & Center for Materials research by Information Integration (CMI^2), Research and Services Division of Materials Data and Integrated System (MaDIS), National Institute for Materials Science (NIMS), Japan	**Informatics-aided DFT-based Solid Electrolyte Search for Rechargeable Battery Application**
29	**Takaki Tokiwa, Mitsuo Shoji, Naoki Shibata, Yoshiki Higuchi, Kunishige Kataoka, Yasuteru Shigeta, Fuminori Misaizu**	Graduate School of Science, Tohoku University, Japan, Graduate School of Pure and Applied Sciences & Center for Computational Sciences, University of Tsukuba, Japan, Graduate School of Life Science, University of Hyogo, Japan	**QM/MM Study on the T1 Cu site structures and the Redox Potentials in Bilirubin Oxidase (BOD)**
30	**Shin Kiyohara, Tomohiro Miyata, Teruyasu Mizoguchi**	Institute of Industrial Science, The University of Tokyo, Japan	**Data driven approaches to reconstruct and interpret**
31	**Ashu Choudhary, Keitaro Sodeyama, Yoshitaka Tateyama**	Center for Green Research on Energy and Environmental Materials (GREEN) & Center for Materials Research by Information Integration (CMI2),, National Institute for Materials Science (NIMS), Japan	**Car-Parrinello Molecular Dynamics (CPMD) Study on Electrolytes based on Grignard Reagents for Magnesium-Ion Battery**
32	**Yu-ichiro Matsushita, Atsushi Oshiyama**	The University of Tokyo, Japan	**Ab initio calculations for interface/near-interface states at SiC/SiO2**
33	**Takuma Kobayashi, Yu-ichiro Matsushita, Tsunenobu Kimoto, Atsushi Oshiyama**	Kyoto University, Japan, The University of Tokyo, Japan	**Microscopic Mechanism of the Removal of Carbon-Associated Defects at a SiO2/SiC Interface due to Phosphorus Treatment**
34	**Yukihiro Okuno, Keisuke Ushirogata, Keitaro Sodeyama, Yoshitaka Tateyama**	Research and Development Management Headquarters, FUJIFILM Corporation, Japan, Center for Green Research on Energy and Environmental Materials (GREEN), National Institute for Materials Science (NIMS), Japan,	**Ab Initio Study on Adsorption Structure and Decomposition Reactions of Electrolytes on the LiNi0.5Mn1.5O4**
35	**Masato Kimatsuka, Yasuteru Shigeta, Mitsuo Shoji**	Graduate School of Pure and Applied Sciences & Center for Computational Sciences, University of Tsukuba, Japan	**Molecular Dynamics Studies on the effects of Anti-Freeze Protein (AFP) on ice growth**
36	**Atsushi Ishikawa, Keitaro Sodeyama, Yoshitaka Tateyama**	JST PRESTO, Japan, Center for Green Research on Energy and Environmental Materials & Center for Materials Research by Information Integration (CMI2), National Institute for Materials Science (NIMS), Japan.	**NO + CO Reaction on Rh Surface: DFT Investigation Combined with Microkinetic Analysis**
38	**Naoyuki Karasawa, Ayori Mitsutake, Hiroshi Takano**	Department of Physics, Faculty of Science and Technology, Keio University, Japan	**Relaxation Mode Analysis of an Erythropoietin and Its Receptors**

39	**F. Muttaqien, H. Oshima, Y. Hamamoto, K. Inagaki, I. Hamada, Y. Morikawa**	Department of Precision Science and Technology, Graduate School of Engineering, Osaka University, Japan	**Formate Decomposition on Cu(111): Importance of CO2 Bending Vibrational Mode**
40	**Sotaro Yamasaki, Mitsuo Shoji, Yasuteru Shigeta**	Graduate School of Pure and Applied Science, University of Tsukuba, Japan	**A QM/MM study on the oxygen-binding structures of alternative oxidase**
41	**M. Kayanuma, M. Shoji, Y. Aikawa, M. Umemura, Y. Shigeta**	Center for Computational Sciences & Graduate School of Pure and Applied Sciences, University of Tsukuba, Japan	**Surface Hopping Simulation on the Photodissociation of Methanol**
42	**Fumihiro Imoto, Jun-Ichi Iwata, Mauro Boero, Atsushi Oshiyama**	Department of Applied Physics, The University of Tokyo, Japan, IPCMS, France	**Initial Formation Mechanisms of Graphene on SiC(0001) Surfaces: Reaction Pathways and Free-Energy Barriers**
43	**Takuro Tsutsumi, Rina Yamamoto, Yu Harabuchi, Tetsuya Taketsugu**	Graduate School of Chemical Sciences and Engineering, Hokkaido University., Japan	**Spin-Flip TDDFT Study of Photoisomarization Dynamics of Monomethyl-stilbene**
44	**Wenwen Li, Yasunobu Ando, Emi Minamitani, Satoshi Watanabe**	Department of Materials Engineering, The University of Tokyo, Japan, Research Center for Computational Design of Advanced Functional Materials (CD-FMat), National Institute of Advanced Industrial Science and Technology (AIST), Japan	**Study of atomic diffusion in amorphous structures using neural network potentials**
45	**Yuta Yamamoto, Tomoharu Motoyama, Vladimir Sladek, Kozmon Stanislav, Shogo Nakano, Shohei Ito, Hiroaki Tokiwa**	Department of Chemistry & Research Center of Smart Molecules, Rikkyo University, Japan, Graduate Division of Nutritional and Environmental Sciences, University of Shizuoka, Japan, Center for Glycomics, Slovak Academy of Sciences, Slovakia	**Computational Study of Enzyme Reaction Mechanism in monomeric L-threonine 3-dehydrogenase**
46	**Mitsuki Togoshi, Satoru. S. Kano, Yasunari Zempo**	Computer and Information Sciences, Hosei University, Japan	**Maximum entropy method applied to TDDFT time-series data**
47	**Masafuyu Matsui1, Shigeyoshi Sakaki**	Element Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, Japan	**Embedded Cluster Model Incorporating Periodic Electrostatic Potential**
48	**Mitsuo Shoji, Hiroshi Isobe, Yasuteru Shigeta, Takahito Nakajima, Kizashi Yamaguchi**	Center for Computational Sciences, University of Tsukuba, Japan, Faculty of Science, Okayama University, Japan, Advanced Institute for Computational Science (AICS), RIKEN, Japan	**QM/MM study on a S4 -> S0 reaction of the Oxygen Evolving Complex in Photosystem II**
49	**Yun-Wen Chen,Jer-Lai Kuo**	Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan	**Ab Initio Study of Water Dissociation on GaN Surfaces**
51	**Minho Kim, Hyung Kyu Lim, Hyungjun Kim**	Graduate School of Energy, Environment, Water and Sustainability (EEWS), Korea Advanced Institute of Science and Technology (KAIST), South Korea	**Grid-based mean-field QM/MM study on the oxygen reduction reaction with classical explicit solvent model**
52	**Dongsun Yoo, Yong Youn, Hochul Song, Seungwu Han**	Department of Materials Science and Engineering and Research Institute of Advanced Materials, Seoul National University, Korea	**Molecular Orientation in Vapor-deposited Organic Semiconductors and Its Effect on Charge Transport**
53	**Taedaehyeong Eom, Hyungjun Kim**	Graduate school of energy, environment, water, and sustainability (EEWS), Korea Advanced institute of Science and technology (KAIST), South Korea	**Modified cluster expansion method for estimating CO2 reduction reaction efficiency**
54	**Pham Tien Lam, Hiori Kino, Dam Hieu Chi**	Japan Advanced Institute of Science and Technology, Japan, Elements Strategy Initiative Center for Magnetic Materials, National Institute for Materials Science, Japan	**Deep Neural network for Learning Pairwise atomic forces**
55	**Jun Haruyama, Minoru Otani**	National Institute of Advanced Industrial Science and Technology (AIST), Japan	**Electrochemical Reaction Simulations at Metal/Water Interfaces Using Density Functional + Implicit Classical Solvation Theory**
56	**So Fujikake, Emi Minamitani, Satoshi Watanabe**	Department of Materials Engineering, The University of Tokyo, Japan	**Thermal Characteristics of Si-Ge Alloy by Machine-Learning Potential**
57	**Minoru Otani**	National Institute of Advanced Industrial Science and Technology (AIST), Japan	**Hybrid DFT/RISM simulation of electrochemical reactions at electrode/electrolyte interface**
58	**Aditya Wibawa Sakti, Yoshifumi Nishimura, Chien-Pin Chou, Hiromi Nakai**	Department of Chemistry and Biochemistry & Research Institute for Science and Engineering, Waseda University, Japan, JST CREST, Japan, Elements Strategy Initiative for Catalysts and Batteries, Kyoto University, Japan	**Fast excess proton diffusion in ice phases: A molecular dynamics study at approximate density-functional level**

59	**J.-I. Iwata, Y. Shigeta, K. Koizumi, M. Boero, A. Oshiyama1**	Department of Applied Physics, The university of Tokyo, Japan, Center for Computational Sciences, University of Tsukuba, Japan, Institute for Molecular Science, Japan, IPCMS, France	**A Real-Space Car-Parrinello Molecular Dynamics (RS-CPMD) simulation code: implementation for massively-parallel and GPGPU supercomputers**
61	**Toshiharu Ohnuma, Takeshi Kobayashi**	Central Research Institute of Electric Power Industry (CRIEPI), Japan	**Na ion diffusion in inorganic solid electrolyte Na4Mg3(PO4)2P2O7**
62	**Yoshiki ISHII, Ryosuke ISHIZUKA, Nobuyuki MATUBAYASI**	Department of Chemical Engineering, Osaka University, Japan	**Atomic Charge Distribution for the Force-Field Development of Ionic Liquids**
63	**Tsuyoshi Miyazaki, David R. Bowler**	International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science (NIMS), Department of Physics and Astronomy & London Centre for Nanotechnology, University College London (UCL), UK	**Million-atom DFT simulations with the CONQUEST code**
64	**Duong-Nguyen NGUYEN, Hieu-Chi DAM, Tien-Lam PHAM**	Japan Advanced Institute of Science and Technology, Japan, Elements Strategy Initiative Center for Magnetic Materials, National Institute for Materials, Japan, JST PRESTO, Japan	**Regression-based feature network construction: unveil the actuation mechanism of Curie temperature**