Michihisa Koyama

List of Publications by Year
in descending order

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198	3,230	172457	206112
papers	citations	29 h-index	48 g-index

202	202	202	3600
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Importance of raw material features for the prediction of flux growth of Al₂O₃ crystals using machine learning. CrystEngComm, 2022, 24, 3179-3188.	2.6	2
2	Techno-economic and life cycle analyses of battery-assisted hydrogen production systems from photovoltaic power. Journal of Cleaner Production, 2021, 298, 126809.	9.3	14
3	Multiyear microgrid data from a research building in Tsukuba, Japan. Scientific Data, 2019, 6, 190020.	5.3	12
4	The effect of SnO2(110) supports on the geometrical and electronic properties of platinum nanoparticles. SN Applied Sciences, 2019, 1, 1.	2.9	13
5	NO Adsorption on 4d and 5d Transition-Metal (Rh, Pd, Ag, Ir, and Pt) Nanoparticles: Density Functional Theory Study and Supervised Learning. Journal of Physical Chemistry C, 2019, 123, 28114-28122.	3.1	22
6	Performance and cost analysis of building scale micro-grid operation. Energy Procedia, 2019, 156, 425-429.	1.8	2
7	Emergence of high ORR activity through controlling local density-of-states by alloying immiscible Au and Ir. Chemical Science, 2019, 10, 652-656.	7.4	50
8	Atomic structure observations and reaction dynamics simulations on triple phase boundaries in solid-oxide fuel cells. Communications Chemistry, 2019, 2, .	4.5	16
9	Theoretical design of a technetium-like alloy and its catalytic properties. Chemical Science, 2019, 10, 5461-5469.	7.4	5
10	How oxides affect the stretching modes of carbon monoxide adsorbed on Ni catalyst?. Applied Surface Science, 2019, 478, 1074-1080.	6.1	5
11	Battery-assisted low-cost hydrogen production from solar energy: Rational target setting for future technology systems. International Journal of Hydrogen Energy, 2019, 44, 1451-1465.	7.1	50
12	Solidâ€Solution Alloy Nanoparticles of the Immiscible Iridiumâ€“Copper System with a Wide Composition Range for Enhanced Electrocatalytic Applications. Angewandte Chemie - International Edition, 2018, 57, 4505-4509.	13.8	86
13	Theoretical Approach to the Sulfidation of the BaTiO₃(001) Surfaces and Its Effect on the H₂ Oxidation Reaction and CH₄ Sequential Dissociation. Journal of Physical Chemistry C, 2018, 122, 1437-1446.	3.1	3
14	Combined theoretical and experimental studies of CO oxidation on PdRu nanoalloys. Applied Catalysis A: General, 2018, 568, 176-182.	4.3	4
15	Influence of inter-particle resistance between active materials on the discharge characteristics of the positive electrode of lithium ion batteries. Electrochimica Acta, 2018, 278, 385-395.	5.2	14
16	First-Principles Study on Oxygen Reduction Reaction over La 1-x Sr x CoO 3-Î´. ECS Transactions, 2017, 77, 75-80.	0.5	2
17	Future energy and electric power systems and smart technologies. IEEJ Transactions on Electrical and Electronic Engineering, 2017, 12, 453-464.	1.4	8
18	Multi-Scale, Multi-Physics Approach for Solid Oxide Fuel Cell Anode Reaction. ECS Transactions, 2017, 78, 2835-2844.	0.5	1

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19	Theoretical Study of Oxygen Vacancy Formation at LSC/GDC Interface. ECS Transactions, 2017, 78, 869-874.	0.5	0
20	Predictive Microkinetic Model for Solid Oxide Fuel Cell Patterned Anode: Based on an Extensive Literature Survey and Exhaustive Simulations. Journal of Physical Chemistry C, 2017, 121, 19069-19079.	3.1	6
21	Structural Stability of Ruthenium Nanoparticles: A Density Functional Theory Study. Journal of Physical Chemistry C, 2017, 121, 27445-27452.	3.1	46
22	Theoretical Study of the Hydrogen Absorption Mechanism into a Palladium Nanocube Coated with a Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2017, 121, 14611-14617.	3.1	23
23	Studies on Interfacial Properties of Electric Double Layer Capacitors in Aqueous Electrolytes by Molecular Dynamics Simulations. Journal of Computer Chemistry Japan, 2017, 16, 112-115.	0.1	0
24	Image contrast enhancement of Ni/YSZ anode during the sliceâ€andâ€view process in FIBâ€SEM. Journal of Microscopy, 2016, 261, 326-332.	1.8	5
25	Present Status of Japanâ€™s Energy. , 2016, , 23-32.		2
26	First-Principles Study on Alloy Nanoparticles for Polymer Electrolyte Fuel Cell Catalyst. ECS Transactions, 2016, 75, 717-721.	0.5	3
27	Density Functional Theory Study for Ni Diffusion on Ni(111) Surface under Solid Oxide Fuel Cell Operating Condition. Journal of Physical Chemistry C, 2016, 120, 16641-16648.	3.1	5
28	A Synthetic Pseudo-Rh: NOx Reduction Activity and Electronic Structure of Pdâ€“Ru Solid-solution Alloy Nanoparticles. Scientific Reports, 2016, 6, 28265.	3.3	44
29	Electronic Structure and Phase Stability of PdPt Nanoparticles. Journal of Physical Chemistry Letters, 2016, 7, 736-740.	4.6	40
30	Theoretical investigation of hydrogen absorption properties of rhodiumâ€“silver alloys. Journal of Alloys and Compounds, 2016, 662, 404-408.	5.5	5
31	Theoretical study on temperature effect of electronic structure and spin state in LaCoO3 by using density functional theory. Solid State Ionics, 2016, 285, 195-201.	2.7	12
32	Analysis of Heat Transfer Mechanism at Hydrophilic/Hydrophobic Surfaces Using Molecular Dynamics Simulation. The Proceedings of Mechanical Engineering Congress Japan, 2016, 2016, J2220306.	0.0	0
33	Future Energy System and Executive Summaries of the Parts. , 2016, , 3-11.		0
34	Theoretical Study of Hydrogen Bonds in Water Nanodroplet on Graphene. Journal of Computer Chemistry Japan, 2016, 15, 85-86.	0.1	0
35	First-Principles Study of Oxygen Transfer and Hydrogen Oxidation Processes at the Ni-YSZ-Gas Triple Phase Boundaries in a Solid Oxide Fuel Cell Anode. Journal of Physical Chemistry C, 2015, 119, 27603-27608.	3.1	17
36	First-principles calculation of OH^{â^'}/OH adsorption on gold nanoparticles. International Journal of Quantum Chemistry, 2015, 115, 1597-1605.	2.0	12

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37	Molecular Dynamics Study on Diffusion Property of Pt Atoms in Ni-Pt Nanoparticle. Journal of Computer Chemistry Japan, 2015, 14, 83-84.	0.1	0
38	Observation of the Ni/YSZ Interface in a Conventional SOFC. Journal of the Electrochemical Society, 2015, 162, F750-F754.	2.9	13
39	B22-P-06Ni/YSZ Interface in A Conventional Solid Oxide Fuel Cell. Microscopy (Oxford, England), 2015, 64, i105.2-i105.	1.5	0
40	Why solid oxide cells can be reversibly operated in solid oxide electrolysis cell and fuel cell modes?. Physical Chemistry Chemical Physics, 2015, 17, 31308-31315.	2.8	63
41	First-principles study of oxygen coverage effect on hydrogen oxidation on Ni(111) surface. Applied Surface Science, 2015, 333, 86-91.	6.1	20
42	Conceptual design of light integrated gasification fuel cell based on thermodynamic process simulation. Applied Energy, 2015, 147, 486-499.	10.1	16
43	A Fundamental Study of Boron Deposition and Poisoning of La_{0.8}Sr_{0.2}MnO₃Cathode of Solid Oxide Fuel Cells under Accelerated Conditions. Journal of the Electrochemical Society, 2015, 162, F1282-F1291.	2.9	13
44	Effect of alloying elements on hydrogen absorption properties of palladium-based solid solution alloys. Journal of Alloys and Compounds, 2015, 653, 444-452.	5.5	14
45	The effects of minor elements in La0.6Sr0.4Co0.2Fe0.8O3-Î´ cathodes on oxygen reduction reaction. Journal of Power Sources, 2015, 277, 44-51.	7.8	9
46	Theoretical study of support effect of Au catalyst for glucose oxidation of alkaline fuel cell anode. Applied Surface Science, 2015, 324, 76-81.	6.1	36
47	Parallel Performance Analysis for Electronic Structure Calculation of Metal Nanoparticles. Journal of Computer Chemistry Japan, 2015, 14, 52-53.	0.1	3
48	Theoretical Analysis of Cation Diffusion Pathway in SOFC Electrolyte. Journal of Computer Chemistry Japan, 2015, 14, 92-93.	0.1	0
49	Density Functional Theory Study of Sulfur Poisoning on Nickel Anode in Solid Oxide Fuel Cells: Effects of Surface and Subsurface Sulfur Atoms. Journal of Chemical Engineering of Japan, 2014, 47, 793-800.	0.6	6
50	Theoretical Study on Interaction Energy between Water and Graphene Model Compounds. Journal of Computer Chemistry Japan, 2014, 13, 171-172.	0.1	4
51	The valence band structure of AgxRh1â€“x alloy nanoparticles. Applied Physics Letters, 2014, 105, .	3.3	27
52	Sintering Simulation for Porous Material by Integrating Molecular Dynamics and Master Sintering Curve. Journal of Physical Chemistry C, 2014, 118, 15766-15772.	3.1	13
53	A scenario analysis of future energy systems based on an energy flow model represented as functionals of technology options. Applied Energy, 2014, 132, 586-601.	10.1	29
54	Microstructure evolution of NiOâ€“YSZ cermet during sintering. Solid State Ionics, 2014, 262, 460-464.	2.7	13

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55	Theoretical study on oxidation reaction mechanism on Au catalyst in direct alkaline fuel cell. Solid State Ionics, 2014, 262, 328-331.	2.7	21
56	Preface to the Special Issue for International Symposium on Innovative Materials for Processes in Energy Systems 2013. Journal of Chemical Engineering of Japan, 2014, 47, 497-497.	0.6	0
57	Present Status and Points of Discussion for Future Energy Systems in Japan from the Aspects of Technology Options. Journal of Chemical Engineering of Japan, 2014, 47, 499-513.	0.6	30
58	OS1610 Theoretical study on the effect of surface adsorbate on Ni surface diffusion. The Proceedings of the Materials and Mechanics Conference, 2014, 2014, _OS1610-1_-_OS1610-2_.	0.0	0
59	Detailed Transport-Reaction Models for SOFC Ni-YSZ Patterned Anodes: A Critical Inquiry. ECS Transactions, 2013, 57, 2821-2830.	0.5	3
60	Detailed Kinetic Modeling for SOFC Ni Pattern Anodes Fuelled by Methane. ECS Transactions, 2013, 57, 2865-2870.	0.5	1
61	Molecular Dynamics Simulation Studies of H Diffusion in SOFC Anode Using Reactive Force Field. ECS Transactions, 2013, 57, 2649-2654.	0.5	3
62	Density Functional Theory Calculation of Spin-State Transition in LaCoO3. ECS Transactions, 2013, 57, 2655-2660.	0.5	2
63	Density Functional Theory Study on the Catalytic Properties of BaTiO3 as Solid Oxide Fuel Cell Anode. ECS Transactions, 2013, 57, 2723-2732.	0.5	2
64	The Effects of Minor Components in LSCF Cathode on Oxygen Reduction Reaction. ECS Transactions, 2013, 57, 1909-1916.	0.5	1
65	Microstructure Observation of Ni/YSZ Boundary by TEM and STEM. ECS Transactions, 2013, 57, 1401-1405.	0.5	3
66	Moleular Dynamics Study for Sintering Property Analysis of Ni-YSZ Cermet. ECS Transactions, 2013, 57, 1407-1413.	0.5	1
67	First-Principles Calculations of the Anodic Oxidation Reactions of Solid Oxide Fuel Cell: Oxygen Potential Effect on Nickel (111) Surface. ECS Transactions, 2013, 57, 2429-2436.	0.5	1
68	A Key Mechanism of Ethanol Electrooxidation Reaction in a Noble-Metal-Free Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2013, 117, 10607-10614.	3.1	29
69	A New Method for Characterization of Porous Structure without Mercury; Application to Porous Materials of Diesel Particulate Filters. , 2013, , .		0
70	Applications of Computational Chemistry to Designing Materials and Microstructure in Fuel Cell Technologies. Journal of Computer Chemistry Japan, 2013, 12, 1-7.	0.1	4
71	A Sense of Reality. Journal of Computer Chemistry Japan, 2013, 12, A25-A25.	0.1	0
72	A Review of Molecular-Level Mechanism of Membrane Degradation in the Polymer Electrolyte Fuel Cell. Membranes, 2012, 2, 395-414.	3.0	48

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73	Molecular dynamics simulation based on the multi-component molecular orbital method: Application to. Chemical Physics, 2012, 392, 166-169.	1.9	7
74	J056041 Theoretical Study on Local Reaction Mechanism of Solid Oxide Fuel Cell Anode. The Proceedings of Mechanical Engineering Congress Japan, 2012, 2012, _J056041-1-_J056041-2.	0.0	0
75	C101 Molecular Dynamics Study on Sintering Properties of Porous Nickel. The Proceedings of the National Symposium on Power and Energy Systems, 2012, 2012.17, 75-76.	0.0	0
76	OS1-2-4 Development of interatomic potential functions for atomistic modeling of solid oxide fuel cell materials. The Proceedings of the Symposium on Micro-Nano Science and Technology, 2012, 2012.4, 165-166.	0.0	0
77	D205 Anodic Reaction Mechanism of Non-Platinum Direct Ethanol Fuel Cell. The Proceedings of the National Symposium on Power and Energy Systems, 2012, 2012.17, 349-350.	0.0	0
78	Theoretical Study on Dissolution and Reprecipitation Mechanism of Pt Complex in Pt Electrocatalyst. Journal of Physical Chemistry C, 2011, 115, 3136-3142.	3.1	10
79	Computational Study on Impurities Poisoning and Degradation of an SOFC Anode Based on Density Functional Theory. ECS Transactions, 2011, 35, 853-858.	0.5	3
80	Stability and hydration structure of model perfluorosulfonic acid compound systems, CF3SO3H(H2O)n (n=1â€“4), and its isotopomer by the direct treatment of H/D nuclear quantum effects. Computational and Theoretical Chemistry, 2011, 975, 92-98.	2.5	9
81	Tackling Power Outages in Japan: The Earthquake Compels a Swift Transformation of the Power Supply. Journal of Chemical Engineering of Japan, 2011, , .	0.6	9
82	Chemical durability of Solid Oxide Fuel Cells: Influence of impurities on long-term performance. Journal of Power Sources, 2011, 196, 9130-9140.	7.8	160
83	Theoretical Study on Chemical Degradation Mechanism of Nafion Side Chain by the Attack of OH Radical in Polymer Electrolyte Fuel Cell. ECS Transactions, 2011, 35, 1-6.	0.5	11
84	Theoretical Study for the Sintering of Nickel Anode in Solid Oxide Fuel Cell. ECS Transactions, 2011, 35, 1661-1667.	0.5	0
85	Applying ultra-accelerated quantum chemical molecular dynamics technique for the evaluation of ligand protein interactions. Medicinal Chemistry Research, 2010, 19, 1-10.	2.4	4
86	The effect of R249S carcinogenic and H168Râ€“R249S suppressor mutations on p53â€“DNA interaction, a multi scale computational study. Computers in Biology and Medicine, 2010, 40, 498-508.	7.0	6
87	Chemical Degradation Mechanism of Model Compound, CF[sub 3](CF[sub 2])[sub 3]O(CF[sub 2])[sub 2]OCF[sub 2]SO[sub 3]H, of PFSA Polymer by Attack of Hydroxyl Radical in PEMFCs. Journal of the Electrochemical Society, 2010, 157, B1305.	2.9	23
88	Quantum Chemistry Study on Absorption Spectra, Electronic and Electrical Properties of Organic Dye on Anatase(001). Journal of Nanoscience and Nanotechnology, 2010, 10, 2434-2443.	0.9	0
89	Tribochemical Reaction Dynamics of Molybdenum Dithiocarbamate on Nascent Iron Surface: A Hybrid Quantum Chemical/Classical Molecular Dynamics Study. Journal of Nanoscience and Nanotechnology, 2010, 10, 2495-2502.	0.9	9
90	Host emission from BaMgAl¹⁰O¹⁷ and SrMgAl¹⁰O¹⁷ phosphor: Effects of temperature and defect level. Journal of the Society for Information Display, 2010, 18, 211-222.	2.1	9

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91	Theoretical Study on Dissoloved Structure of Pt Complex in Polymer Electrolyte Fuel Cell. ECS Transactions, 2009, 25, 799-806.	0.5	2
92	Simulation of Electron Diffusion in TiO2Porous Structures in Dye-Sensitized Solar Cells. Japanese Journal of Applied Physics, 2009, 48, 04C166.	1.5	11
93	The Effect of Particle Size on the Microstructure and the Effective Reaction Zone of SOFC Cermet Anodes. ECS Transactions, 2009, 16, 229-234.	0.5	2
94	Novel Method Based on Quantum Chemistry for Calculation of Ion Induced Secondary Electron Emission Coefficient of MgO Surfaces. Japanese Journal of Applied Physics, 2009, 48, 04C145.	1.5	0
95	A Theoretical Study of Initial Deposition Processes of Mg on MgO: A Novel Quantum Chemical Molecular Dynamics Approach. Japanese Journal of Applied Physics, 2009, 48, 04C126.	1.5	3
96	Theoretical Study for Properties of SOFC Anode Using Three-Dimensional Porous Structure Simulator. ECS Transactions, 2009, 25, 1847-1853.	0.5	1
97	Ultra Accelerated Quantum Chemical Molecular Dynamics Study on Ethylene Polymerization Reaction Using CpSiH2NHTiCl2â€"Constrained Geometry Catalyst. Topics in Catalysis, 2009, 52, 724-730.	2.8	2
98	Development and Application of Sintering Dynamics Simulation for Automotive Catalyst. Topics in Catalysis, 2009, 52, 1852-1855.	2.8	7
99	A DFT study on the carbamates formation through the absorption of CO2 by AMP. International Journal of Greenhouse Gas Control, 2009, 3, 612-616.	4.6	43
100	An electrical conductivity prediction simulator based on TB-QCMD and KMC. System development and applications. Computational and Theoretical Chemistry, 2009, 903, 11-22.	1.5	5
101	Quantum chemical studies for oxidation of morpholine by Cytochrome P450. Journal of Inorganic Biochemistry, 2009, 103, 20-27.	3.5	12
102	Enhanced gas-sensing behaviour of Ru-doped SnO2 surface: A periodic density functional approach. Journal of Physics and Chemistry of Solids, 2009, 70, 1248-1255.	4.0	44
103	Influence of nanometer scale film structure of ZDDP tribofilm on Its mechanical properties: A computational chemistry study. Applied Surface Science, 2009, 256, 976-979.	6.1	14
104	A graph theoretical approach to the effect of mutation on the flexibility of the DNA binding domain of p53 protein. Chemical Papers, 2009, 63, .	2.2	2
105	19.3: Electronic Structure Calculation and QSPR Analysis of Eu²⁺â€doped Oxide Phosphors: Relationship between Emission Wavelength and Crystal Structure. Digest of Technical Papers SID International Symposium, 2009, 40, 254-257.	0.3	0
106	Dynamics of Hydrogen Spillover on Pt/Î³-Al2O3 Catalyst Surface: A Quantum Chemical Molecular Dynamics Study. Journal of Physical Chemistry C, 2009, 113, 15676-15683.	3.1	64
107	A Computational Chemistry Study on Friction of h-MoS₂. Part I. Mechanism of Single Sheet Lubrication. Journal of Physical Chemistry B, 2009, 113, 16526-16536.	2.6	165
108	A DFT Study for the Durability of Perfluorosulfonic Acid Membrane. ECS Transactions, 2009, 25, 765-772.	0.5	4

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109	Study of Carbon Monoxide Oxidation on CeO₂(111) Using Ultra Accelerated Quantum Chemical Molecular Dynamics. Journal of Physical Chemistry C, 2009, 113, 7723-7727.	3.1	34
110	Theoretical investigation of ethylene/1-butene copolymerization process using constrained geometry catalyst (CpSiH2NH)-Ti-Cl2. Applied Surface Science, 2008, 254, 7608-7611.	6.1	10
111	Development of a new molecular dynamics method for tribochemical reaction and its application to formation dynamics of MoS2 tribofilm. Applied Surface Science, 2008, 254, 7618-7621.	6.1	71
112	Development of porous structure simulator for multi-scale simulation of irregular porous catalysts. Applied Surface Science, 2008, 254, 7774-7776.	6.1	10
113	Development of the reaction time accelerating molecular dynamics method for simulation of chemical reaction. Applied Surface Science, 2008, 254, 7955-7958.	6.1	5
114	A theoretical investigation on the abrasive wear prevention mechanism of ZDDP and ZP tribofilms. Applied Surface Science, 2008, 254, 7976-7979.	6.1	19
115	Development of the overpotential simulator for polymer electrolyte fuel cells and application for optimization of cathode structure. Applied Surface Science, 2008, 254, 7929-7932.	6.1	29
116	Internet-Based Integrated Environmental Assessment, Part II: Semantic Searching Based on Ontologies and Agent Systems for Knowledge Discovery. Journal of Industrial Ecology, 2008, 10, 37-60.	5.5	15
117	Computational Evaluation of Electrical Conductivity on SiC and the Influence of Crystal Defects. Materials Science Forum, 2008, 600-603, 497-500.	0.3	3
118	Theoretical Study on Electronic and Electrical Properties of Nanostructural ZnO. Japanese Journal of Applied Physics, 2008, 47, 2999.	1.5	24
119	Influence of Organic Functional Groups on the Electrical Properties of Carbon Black: A Theoretical Study. Japanese Journal of Applied Physics, 2008, 47, 3147-3151.	1.5	3
120	Development of A Seebeck Coefficient Prediction Simulator Using Tight-Binding Quantum Chemical Molecular Dynamics. Japanese Journal of Applied Physics, 2008, 47, 3134-3137.	1.5	3
121	Development of Multiscale Simulator for Dye-Sensitized TiO2Nanoporous Electrode Based on Quantum Chemical Calculation. Japanese Journal of Applied Physics, 2008, 47, 3010-3014.	1.5	10
122	Effect of Surface Termination on Superlow Friction of Diamond Film: A Theoretical Study. Japanese Journal of Applied Physics, 2008, 47, 3032-3035.	1.5	22
123	A Theoretical Investigation on the Dynamic Behavior of Molybdenum Dithiocarbamate Molecule in the Engine Oil Phase. Tribology Online, 2008, 3, 80-85.	0.9	16
124	Multi-scale Simulation Approach for Polymer Electrolyte Fuel Cell Cathode Design. ECS Transactions, 2008, 16, 57-66.	0.5	2
125	A Theoretical Study of Dynamic Behavior of Diphenyldisulphide Molecule on Fe Surface: Novel Ultra-Accelerated Quantum Chemical Molecular Dynamics Approach. Tribology Online, 2008, 3, 280-284.	0.9	15
126	Development of Three-Dimensional Porous Structure Simulator POCO2 for Simulations of Irregular Porous Materials. Journal of Computer Chemistry Japan, 2008, 7, 55-62.	0.1	13

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127	Theoretical Simulation of Dielectric Breakdown by Molecular Dynamics and Tight-Binding Quantum Chemistry Methods. Japanese Journal of Applied Physics, 2007, 46, 1853-1858.	1.5	6
128	Development of Three-Dimensional Porous Structure Simulator for Optimizing Microstructure of SOFC Anode. ECS Transactions, 2007, 7, 2057-2064.	0.5	11
129	Combinatorial Computational Chemistry Approach for Materials Design:Applications in deNOx Catalysis, Fischer-Tropsch Synthesis, Lanthanoid Complex, and Lithium Ion Secondary Battery. Combinatorial Chemistry and High Throughput Screening, 2007, 10, 99-110.	1.1	9
130	Development of Constraint Algorithm for the Number of Electrons in Molecular Orbitals Consisting Mainly 4fAtomic Orbitals of Rare-Earth Elements and Its Introduction to Tight-Binding Quantum Chemical Molecular Dynamics Method. Japanese Journal of Applied Physics, 2007, 46, 2505-2509.	1.5	8
131	Large-Scale Electronic Structure Calculation on Blue Phosphor BaMgAl10O17:Eu2+Using Tight-Binding Quantum Chemistry Method Implemented for Rare-Earth Elements. Japanese Journal of Applied Physics, 2007, 46, 2534-2541.	1.5	12
132	Development of a Thermal Conductivity Prediction Simulators Based on the Effects of Electron Conduction and Lattice Vibration. Japanese Journal of Applied Physics, 2007, 46, 2609-2614.	1.5	4
133	Theoretical Study on the Electronic and Electrical Properties of p-Type Transparent Conducting Metal Oxides. Japanese Journal of Applied Physics, 2007, 46, 2603-2608.	1.5	2
134	Theoretical Investigation on Electrical and Electronic Properties of Carbon Materials. Japanese Journal of Applied Physics, 2007, 46, 2650-2654.	1.5	5
135	Theoretical Investigation of the Photophysical Properties of Black Dye Sensitizer [(H3-tctpy)M(NCS)3]-(M = Fe, Ru, Os) in Dye Sensitized Solar Cells. Japanese Journal of Applied Physics, 2007, 46, 2655-2660.	1.5	11
136	Theoretical Study on the ATP Hydrolysis Mechanism of HisP Protein, the ATP-Binding Subunit of ABC Transporter. Materials Transactions, 2007, 48, 735-739.	1.2	1
137	A DFT Study of the Heme Role in the N-Demethylation of Theophylline Mediated by Compound I of Cytochrome P450. Materials Transactions, 2007, 48, 730-734.	1.2	3
138	Does Metabolism of (<I>S</I>)-<I>N</I>-[1-(3-Morpholin-4-ylphenyl)ethyl]-3-phenylacrylamide Occur at the Morpholine Ring? Quantum Mechanical and Molecular Dynamics Studies. Materials Transactions, 2007, 48, 740-744.	1.2	1
139	Electronic structure and electrical conductivity of MgO protecting layer in plasma-display panels: A tight-binding quantum chemical study. Journal of the Society for Information Display, 2007, 15, 307.	2.1	2
140	Novel computational chemistry approaches for studying physico-chemical properties of zeolite materials. Microporous and Mesoporous Materials, 2007, 101, 324-333.	4.4	7
141	Oxidation mechanism in the metabolism of (S)-N-[1-(3-morpholin-4-ylphenyl)ethyl]-3-phenylacrylamide on oxyferryl active site in CYP3A4 Cytochrome: DFT modeling. Journal of Molecular Modeling, 2007, 13, 851-860.	1.8	6
142	Theoretical Study on Electronic and Electrical Properties of Nano Structural ZnO. , 2007, , .		0
143	Development of the multi-scale simulator for the dye-sensitized TiO2 nanoporous electrode based on quantum chemical calculation. , 2007, , .		0
144	Tight-Binding Quantum Chemical Molecular Dynamics Study on First Proton Transfer Process of ORR Catalyzed by Cobalt-Porphyrin Complex. Electrochemical and Solid-State Letters, 2006, 9, A490.	2.2	21

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145	First-Principles Study on Proton Dissociation Properties of Fluorocarbon- and Hydrocarbon-Based Membranes in Low Humidity Conditions. Journal of Physical Chemistry B, 2006, 110, 17872-17877.	2.6	18
146	Tribochemical Reaction Dynamics of Phosphoric Ester Lubricant Additive by Using a Hybrid Tight-Binding Quantum Chemical Molecular Dynamics Method. Journal of Physical Chemistry B, 2006, 110, 17507-17511.	2.6	54
147	Model first principles molecular dynamics study on the fate of vibrationally excited states in liquid water. Molecular Physics, 2006, 104, 2093-2100.	1.7	0
148	Combinatorial computational chemistry: first principles quantum methods as a tool for industrial innovations. Studies in Surface Science and Catalysis, 2006, 159, 9-16.	1.5	0
149	Interfacial properties of ZrO2 supported precious metal catalysts: A density functional study. Applied Catalysis A: General, 2006, 305, 102-109.	4.3	24
150	Molecular dynamics study on the ligand recognition by tandem SH3 domains of p47phox, regulating NADPH oxidase activity. Computational Biology and Chemistry, 2006, 30, 303-312.	2.3	6
151	Hyperconjugation with lone pair of morpholine nitrogen stabilizes transition state for phenyl hydroxylation in CYP3A4 metabolism of (S)-N-[1-(3-morpholin-4-yl phenyl) ethyl]-3-phenylacrylamide. Chemical Physics Letters, 2006, 419, 523-527.	2.6	7
152	CO2-emissions reduction potential and costs of a decentralized energy system for providing electricity, cooling and heating in an office-building in Tokyo. Energy, 2006, 31, 3041-3061.	8.8	42
153	Combinatorial computational chemistry approach of tight-binding quantum chemical molecular dynamics method to the design of the automotive catalysts. Applied Surface Science, 2006, 252, 2598-2602.	6.1	9
154	Investigation of charge transfer and structural distortions during photo-inducted excitation of cuprous bis-2,9-dimethyl-1,10-phenanthroline complex by density functional theory. Journal of Organometallic Chemistry, 2006, 691, 551-556.	1.8	14
155	A density functional investigation of charge transfer and structural distortions of cuprous(I) bis-phenanthroline under photo-induced excitation. Journal of Photochemistry and Photobiology A: Chemistry, 2006, 179, 149-155.	3.9	14
156	Periodic density functional and tight-binding quantum chemical molecular dynamics study of catalytic properties on Î³-Al2O3 supported Pt catalysts. Applied Catalysis A: General, 2006, 305, 64-69.	4.3	28
157	Three-dimensional quantitative structureâ€“activity relationship (3 D-QSAR) and docking studies on (benzothiazole-2-yl) acetonitrile derivatives as c-Jun N-terminal kinase-3 (JNK3) inhibitors. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 5917-5925.	2.2	31
158	Different support effect of M/ZrO2 and M/CeO2 (M=Pd and Pt) catalysts on CO adsorption: A periodic density functional study. Catalysis Today, 2006, 111, 322-327.	4.4	38
159	H-MOR: Density functional investigation for the relative strength of BrÃ¸nsted acid sites and dynamics simulation of NH3 protonationâ€“deprotonation. Journal of Molecular Catalysis A, 2006, 243, 1-7.	4.8	16
160	Development of Hybrid Tight-Binding Quantum Chemical Molecular Dynamics Method and Its Application to Boron Implantation into Preamorphized Silicon Substrate. Japanese Journal of Applied Physics, 2006, 45, 2970-2974.	1.5	14
161	Development of Electrical Conductivity Estimation Method Based on Tight-Binding Quantum Chemical Molecular Dynamics Simulation. Japanese Journal of Applied Physics, 2006, 45, 3137-3143.	1.5	15
162	A Theoretical Study of the Effect of Eu ion Dopant on the Electronic Excitations of Yttrium Oxide and Yttrium Oxy-Sulphide. Japanese Journal of Applied Physics, 2006, 45, 5782-5785.	1.5	3

#	Article	IF	Citations
163	COMPUTATIONAL CHEMISTRY FOR INDUSTRIAL INNOVATION. Reviews in Chemical Engineering, 2006, 22, .	4.4	18
164	An Emergent Simulation Modeling Approach for Discovery of Knowledge on Phenomena in Chemical Systems. Journal of Chemical Engineering of Japan, 2006, 39, 1010-1027.	0.6	4
165	Theoretical Investigation of Electrical and Electronic Properties of Carbon Materials. , 2006, , .		0
166	Theoretical Simulation of Dielectric Breakdown by Molecular Dynamics and Tight-Binding Quantum Chemistry Methods. , 2006, , .		0
167	Molecular Dynamics Study on the Activation Mechanism of p47phox in the Auto-Inhibited Form. Journal of Computer Chemistry Japan, 2006, 5, 81-92.	0.1	0
168	Tight-binding quantum chemical molecular dynamics simulation of mechano-chemical reactions during chemicalâ€“mechanical polishing process of SiO2 surface by CeO2 particle. Applied Surface Science, 2005, 244, 34-38.	6.1	75
169	Development of new kinetic Monte Carlo simulator for hydrogen diffusion process in palladiumâ€“silver alloys. Applied Surface Science, 2005, 244, 636-639.	6.1	9
170	Computational chemistry study of solid and aqueous solution interface. Applied Surface Science, 2005, 244, 640-643.	6.1	8
171	Periodic density functional investigation of Lewis acid sites in zeolites: relative strength order as revealed from NH3 adsorption. Applied Surface Science, 2005, 246, 96-101.	6.1	26
172	Tight-binding quantum chemical molecular dynamics method: a novel approach to the understanding and design of new materials and catalysts. Catalysis Today, 2005, 100, 11-25.	4.4	16
173	Theoretical study on the electronic and molecular properties of ground and excited states of ethylenedioxythiophene and styrenesulphonic acid. Applied Surface Science, 2005, 244, 195-198.	6.1	19
174	Photocatalytic oxidation dynamics of acetone on TiO2: tight-binding quantum chemical molecular dynamics study. Applied Surface Science, 2005, 244, 541-545.	6.1	14
175	Tight-binding quantum chemical molecular dynamics simulation of boron activation process in crystalline silicon. Applied Surface Science, 2005, 244, 30-33.	6.1	1
176	Large-scale calculations of solid oxide fuel cell cermet anode by tight-binding quantum chemistry method. Applied Surface Science, 2005, 244, 598-602.	6.1	9
177	Density functional theory studies on decomposition of ethyl-palladium complexes: an important role of cationic species. Applied Surface Science, 2005, 244, 631-635.	6.1	5
178	Periodic density functional and tight-binding quantum chemical molecular dynamics study of surface hydroxyl groups on ZrO2(111)-supported Pt catalyst. Applied Surface Science, 2005, 244, 644-647.	6.1	4
179	Internet-Based Integrated Environmental Assessment Using Ontologies to Share Computational Models. Journal of Industrial Ecology, 2005, 9, 31-50.	5.5	31
180	A flexible model integration approach for evaluating tradeoffs between CO2 emissions and cost in solid oxide fuel cell-based building energy systems. International Journal of Energy Research, 2005, 29, 1261-1278.	4.5	5

#	Article	IF	Citations
181	Tight-Binding Quantum Chemical Molecular Dynamics Method: a Novel Approach to the Understanding and Design of New Materials and Catalysts. ChemInform, 2005, 36, no.	0.0	0
182	A theoretical investigation of the photo-induced intramolecular charge transfer excitation of cuprous (I) bis-phenanthroline by density functional theory. Journal of Organometallic Chemistry, 2005, 690, 187-192.	1.8	8
183	Tight-Binding Quantum Chemical Molecular Dynamics Study on Depth Profile Prediction in Low Energy Boron Implantation Process. Japanese Journal of Applied Physics, 2005, 44, 2288-2293.	1.5	8
184	Tight-Binding Quantum Chemical Calculations of Electronic Structures of Indium Tin Oxide. Japanese Journal of Applied Physics, 2005, 44, 2806-2809.	1.5	10
185	Pharmacokinetic simulator with three-dimensional graphical models: Sociotechnological interface of pharmacokinetics for medical personnel, patients, and medicinal chemists. International Congress Series, 2005, 1284, 296-301.	0.2	0
186	Integrated model framework for the evaluation of an SOFC/GT system as a centralized power source. International Journal of Energy Research, 2004, 28, 13-30.	4.5	29
187	A modularized framework for solving an economicâ€“environmental power generation mix problem. International Journal of Energy Research, 2004, 28, 769-784.	4.5	8
188	Periodic density functional investigation of BrÃ¸nsted acidity in isomorphously substituted chabazite and AlPO-34 molecular sieves. Microporous and Mesoporous Materials, 2004, 71, 51-56.	4.4	35
189	Scenarios of solid oxide fuel cell introduction into Japanese society. Journal of Power Sources, 2004, 131, 327-339.	7.8	33
190	Ligand effect on the periodic properties of trivalent organolanthanide complexes: a density functional study. Inorganic Chemistry Communication, 2004, 7, 566-568.	3.9	6
191	Theoretical Calculations on Electronic Structure and Catalytic Reaction of Organo-f-element Complexes. Chemistry Letters, 2004, 33, 780-785.	1.3	16
192	Dynamics of water and methanol in h-mordenite. Studies in Surface Science and Catalysis, 2004, 154, 2143-2150.	1.5	0
193	Object-based modeling of SOFC system: dynamic behavior of micro-tube SOFC. Journal of Power Sources, 2003, 118, 430-439.	7.8	97
194	Analysis of the Anodic Reaction Mechanism for Solid Oxide Fuel Cell Using BaCeO3 Electrolyte.. Kagaku Kogaku Ronbunshu, 2003, 29, 214-220.	0.3	3
195	The Mechanism of Porous Sm[sub 0.5]Sr[sub 0.5]CoO[sub 3] Cathodes Used in Solid Oxide Fuel Cells. Journal of the Electrochemical Society, 2001, 148, A795.	2.9	131
196	Reaction model of dense Sm0.5Sr0.5CoO3 as SOFC cathode. Solid State Ionics, 2000, 132, 279-285.	2.7	183
197	La[sub 0.6]Ba[sub 0.4]CoO[sub 3] as a Cathode Material for Solid Oxide Fuel Cells Using a BaCeO[sub 3] Electrolyte. Journal of the Electrochemical Society, 2000, 147, 87.	2.9	35
198	Multi-Level Simulation Study of Crystal Growth and Defect Formation Processes in SiC. Materials Science Forum, 0, 600-603, 131-134.	0.3	0