Momoji Kubo

List of Publications by Year
in descending order

369 papers	6,159 citations	76326 40 h-index	149698 56 g-index
374 all docs	374 docs citations	374 times ranked	4601 citing authors

#	Article	IF	Citations
1	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
2	A Computational Chemistry Study on Friction of h-MoS₂. Part II. Friction Anisotropy. Journal of Physical Chemistry B, 2010, 114, 15832-15838.	2.6	121
3	A Quantum Molecular Dynamics Simulation Study of the Initial Hydrolysis Step in Solâ^'Gel Process. Journal of Physical Chemistry B, 2003, 107, 1518-1524.	2.6	115
4	Grand canonical Monte Carlo simulation of the adsorption of CO2 on silicalite and NaZSM-5. Applied Surface Science, 1997, 120, 81-84.	6.1	103
5	Tribochemical Reaction Dynamics Simulation of Hydrogen on a Diamond-like Carbon Surface Based on Tight-Binding Quantum Chemical Molecular Dynamics. Journal of Physical Chemistry C, 2011, 115, 22981-22986.	3.1	95
6	NH3 Adsorption on the BrÃ¶nsted and Lewis Acid Sites of V2O5(010):â€‰ A Periodic Density Functional Study. Journal of Physical Chemistry B, 1999, 103, 4701-4706.	2.6	92
7	Diamond-like carbon coating under oleic acid lubrication: Evidence for graphene oxide formation in superlow friction. Scientific Reports, 2017, 7, 46394.	3.3	90
8	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
9	Effect of Tribochemical Reaction on Transfer-Film Formation by Poly(tetrafluoroethylene). Journal of Physical Chemistry C, 2014, 118, 11820-11826.	3.1	73
10	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
11	Triboemission of hydrocarbon molecules from diamond-like carbon friction interface induces atomic-scale wear. Science Advances, 2019, 5, eaax9301.	10.3	70
12	Friction Reduction Mechanism of Hydrogen- and Fluorine-Terminated Diamond-Like Carbon Films Investigated by Molecular Dynamics and Quantum Chemical Calculation. Journal of Physical Chemistry C, 2012, 116, 12559-12565.	3.1	67
13	Density functional theory analysis of methanation reaction of CO2 on Ru nanoparticle supported on TiO2 (101). Applied Catalysis A: General, 2014, 470, 405-411.	4.3	67
14	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
15	Development of RYUGA for three-dimensional dynamic visualization of molecular dynamics results. Catalysis Today, 1995, 23, 409-416.	4.4	59
16	Study of the Activity of Ga-ZSM-5 in the de-NOx Process by a Combination of Quantum Chemistry, Molecular Dynamics, and Computer Graphics Methods. The Journal of Physical Chemistry, 1995, 99, 12461-12465.	2.9	58
17	Structure and Function of Transfer Film Formed from PTFE/PEEK Polymer Blend. Journal of Physical Chemistry C, 2017, 121, 14589-14596.	3.1	58
18	Density functional theory calculations of the reaction pathway for methane activation on a gallium site in metal exchanged ZSMâ€5. Journal of Chemical Physics, 1995, 103, 2102-2108.	3.0	57

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19	Periodic density-functional study on oxidation of diamond (100) surfaces. Physical Review B, 2000, 61, 11025-11033.	3.2	55
20	Theoretical Investigation on Functionalization of Alkanes by a Rhodium Complex Catalyst. Organometallics, 2002, 21, 3703-3708.	2.3	54
21	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
22	Molecular Dynamics Simulation of Ni Nanoparticles Sintering Process in Ni/YSZ Multi-Nanoparticle System. Journal of Physical Chemistry C, 2013, 117, 9663-9672.	3.1	54
23	Molecular dynamics simulation of enhanced oxygen ion diffusion in strained yttria-stabilized zirconia. Applied Physics Letters, 1998, 73, 1502-1504.	3.3	52
24	Chemical Reaction Mechanism of Polytetrafluoroethylene on Aluminum Surface under Friction Condition. Journal of Physical Chemistry C, 2014, 118, 5390-5396.	3.1	52
25	Tribochemical reactions and graphitization of diamond-like carbon against alumina give volcano-type temperature dependence of friction coefficients: A tight-binding quantum chemical molecular dynamics simulation. Carbon, 2018, 133, 350-357.	10.3	52
26	Periodic density functional study on V2O5 bulk and (001) surface. Applied Surface Science, 1998, 130-132, 539-544.	6.1	49
27	Atomic control of layer-by-layer epitaxial growth onSrTiO3(001):Molecular-dynamics simulations. Physical Review B, 1997, 56, 13535-13542.	3.2	48
28	Molecular dynamics simulation of iso- and n-butane permeations through a ZSM-5 type silicalite membrane. Journal of Membrane Science, 1997, 134, 127-139.	8.2	48
29	Adsorption of H2O on the V2O5(010) Surface Studied by Periodic Density Functional Calculations. Journal of Physical Chemistry B, 1999, 103, 3218-3224.	2.6	48
30	Molecular Dynamics Simulation of Friction of Hydrocarbon Thin Films. Langmuir, 1999, 15, 7816-7821.	3.5	48
31	Electronic structures and spectroscopic properties of dimers Cu2, Ag2, and Au2 calculated by density functional theory. Computational and Theoretical Chemistry, 2002, 579, 221-227.	1.5	47
32	Experimental and Molecular Dynamics Simulations of Tribochemical Reactions with ZDDP: Zinc Phosphateâ€“Iron Oxide Reaction. Tribology Transactions, 2008, 51, 589-601.	2.0	45
33	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
34	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
35	Tight-Binding Quantum Chemical Molecular Dynamics Study on the Friction and Wear Processes of Diamond-Like Carbon Coatings: Effect of Tensile Stress. ACS Applied Materials & Interfaces, 2017, 9, 34396-34404.	8.0	43
36	Homoepitaxial growth mechanism of ZnO(0001): Molecular-dynamics simulations. Physical Review B, 2000, 61, 16187-16192.	3.2	42

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37	Atomistic Mechanisms of Chemical Mechanical Polishing of a Cu Surface in Aqueous H₂O₂: Tight-Binding Quantum Chemical Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2016, 8, 11830-11841.	8.0	42
38	On the electronic structure of the palladium monoxide and the methane adsorption: Density functional calculations. Journal of Chemical Physics, 1996, 104, 4098-4104.	3.0	40
39	Density functional study on the activation of methane over Pd2, PdO, and Pd2O clusters. International Journal of Quantum Chemistry, 1997, 61, 673-682.	2.0	40
40	Quantum Chemical Molecular Dynamics Simulation of the Plasma Etching Processes. Japanese Journal of Applied Physics, 2003, 42, 1859-1864.	1.5	40
41	Transfer-Film Formation Mechanism of Polytetrafluoroethylene: A Computational Chemistry Approach. Journal of Physical Chemistry C, 2013, 117, 10464-10472.	3.1	40
42	Tight-binding quantum chemical molecular dynamics simulations of the low friction mechanism of fluorine-terminated diamond-like carbon films. RSC Advances, 2014, 4, 33739.	3.6	40
43	The distribution of framework aluminum atoms and extraframework exchanged cations in faujasite as studied by molecular dynamics, NMR simulation, neutron diffraction simulation and computer graphics. Microporous Materials, 1996, 7, 235-242.	1.6	39
44	Development of New Tight-Binding Molecular Dynamics Program to Simulate Chemical-Mechanical Polishing Processes. Japanese Journal of Applied Physics, 2002, 41, 2410-2413.	1.5	39
45	Selective T-site substitution as a cause of the anisotropy of lattice expansion in titanosilicate-1 investigated by molecular dynamics and computer graphics. Microporous Materials, 1995, 4, 53-57.	1.6	38
46	Permeation dynamics of small molecules through silica membranes: Molecular dynamics study. AIChE Journal, 1998, 44, 1335-1343.	3.6	38
47	Reactivity of Lattice Oxygens Present in V2O5(010):â€‰ A Periodic First-Principles Investigation. Journal of Physical Chemistry B, 1999, 103, 1263-1269.	2.6	38
48	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
49	First-principle study on reactions of diamond (100) surfaces with hydrogen and methyl radicals. Physical Review B, 2000, 62, 16995-17003.	3.2	37
50	Combinatorial computational chemistry approach to the design of deNOx catalysts. Applied Catalysis A: General, 2000, 194-195, 183-191.	4.3	36
51	Deformation and Fracture Processes of a Lamellar Structure in Polyethylene at the Molecular Level by a Coarse-Grained Molecular Dynamics Simulation. Macromolecules, 2017, 50, 3690-3702.	4.8	36
52	Ring Opening of Methylenecyclopropane over Lanthanocene Catalyst:â€‰ A Quantum-Chemical Molecular Dynamics Simulation Study. Organometallics, 2003, 22, 2181-2183.	2.3	35
53	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
54	Proposal of a new formation mechanism for hydrogenated diamond-like carbon transfer films: Hydrocarbon-emission-induced transfer. Carbon, 2019, 154, 7-12.	10.3	35

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55	Combinatorial computational chemistry approach as a promising method for design of Fischerâ€“Tropsch catalysts based on Fe and Co. Applied Surface Science, 2002, 189, 245-252.	6.1	34
56	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
57	Fate of methanol molecule sandwiched between hydrogen-terminated diamond-like carbon films by tribochemical reactions: tight-binding quantum chemical molecular dynamics study. Faraday Discussions, 2012, 156, 137.	3.2	33
58	Electronic structure and adsorption properties of precious metals and their oxides: Density functional calculations. Journal of Molecular Catalysis A, 1997, 119, 35-44.	4.8	32
59	Fracture Process of Double-Network Gels by Coarse-Grained Molecular Dynamics Simulation. Macromolecules, 2018, 51, 3075-3087.	4.8	32
60	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
61	Ionic Conductivity in Ionic Liquid Nano Thin Films. ACS Nano, 2018, 12, 10509-10517.	14.6	31
62	Structural Properties of LixMn2O4as Investigated by Molecular Dynamics and Density Functional Theory. Japanese Journal of Applied Physics, 2000, 39, 4318-4322.	1.5	30
63	Contrasting Roles of Water at Sliding Interfaces between Silicon-Based Materials: First-Principles Molecular Dynamics Sliding Simulations. Journal of Physical Chemistry C, 2018, 122, 10459-10467.	3.1	30
64	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
65	Development of tight-binding, chemical-reaction-dynamics simulator for combinatorial computational chemistry. Applied Surface Science, 2004, 223, 188-195.	6.1	28
66	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
67	Nanoscratching of multi-layer graphene by molecular dynamics simulations. Tribology International, 2015, 88, 85-88.	5.9	28
68	Quantum chemical study on the oxidation process of a hydrogen terminated Si surface. Journal of Chemical Physics, 1998, 109, 1495-1504.	3.0	27
69	Molecular dynamics calculations of CO2/N2 mixture through the NaY type zeolite membrane. Journal of Membrane Science, 2001, 188, 21-28.	8.2	27
70	A density functional theory calculation on lanthanide monosulfides. Chemical Physics, 2002, 282, 197-206.	1.9	27
71	Tribocatalytic Reaction of Polytetrafluoroethylene Sliding on an Aluminum Surface. Journal of Physical Chemistry C, 2015, 119, 15954-15962.	3.1	27
72	Mechanism of Layer-by-Layer Homoepitaxial Growth of SrTiO3(100) as Investigated by Molecular Dynamics and Computer Graphics. Japanese Journal of Applied Physics, 1992, 31, 4463-4464.	1.5	26

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73	Mechanism of the formation of ultrafine gold particles on MgO(100) as investigated by molecular dynamics and computer graphics. Applied Surface Science, 1995, 89, 131-139.	6.1	26
74	Comparative Investigation on the Adsorption Properties of Precious Metal Clusters toward NO:Â A Density Functional Study. Journal of Physical Chemistry B, 2000, 104, 5110-5117.	2.6	26
75	Quantum Chemical Calculations of Sulfur Doping Reactions in Diamond CVD. Japanese Journal of Applied Physics, 2001, 40, 2830-2832.	1.5	26
76	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
77	Tight-binding Molecular Dynamics Simulation of Desorbed SiO Molecule during the Oxidation of Si(111) Surface. Japanese Journal of Applied Physics, 1999, 38, 2434-2437.	1.5	24
78	Materials design of perovskite-based oxygen ion conductor by molecular dynamics method. Solid State Ionics, 2003, 160, 93-101.	2.7	24
79	Interfacial properties of ZrO2 supported precious metal catalysts: A density functional study. Applied Catalysis A: General, 2006, 305, 102-109.	4.3	24
80	Theoretical Study on Electronic and Electrical Properties of Nanostructural ZnO. Japanese Journal of Applied Physics, 2008, 47, 2999.	1.5	24
81	Self-Formed Double Tribolayers Play Collaborative Roles in Achieving Superlow Friction in an Aqueous Environment. Journal of Physical Chemistry C, 2020, 124, 8295-8303.	3.1	24
82	Layer-by-layer homoepitaxial growth process of MgO(001) as investigated by molecular dynamics, density functional theory, and computer graphics. Journal of Chemical Physics, 1997, 107, 4416-4422.	3.0	23
83	Atomically mixed Fe-group nanoalloys: catalyst design for the selective electrooxidation of ethylene glycol to oxalic acid. Physical Chemistry Chemical Physics, 2015, 17, 11359-11366.	2.8	23
84	Tight-Binding Molecular Dynamics Study of Hydrogen Molecule Inside Silicon Crystal. Japanese Journal of Applied Physics, 2000, 39, 2744-2747.	1.5	22
85	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
86	Development of a Transferable ReaxFF Parameter Set for Carbon- and Silicon-Based Solid Systems. Journal of Physical Chemistry C, 2020, 124, 10007-10015.	3.1	22
87	Molecular dynamics simulation of traction fluid molecules under EHL condition. Thin Solid Films, 1996, 281-282, 598-601.	1.8	21
88	Title is missing!. Topics in Catalysis, 2000, 11/12, 271-278.	2.8	21
89	Quantum-chemical study on the supported precious metal catalyst. Catalysis Today, 2003, 87, 43-50.	4.4	21
90	A study on the excitations of ligand-to-metal charge transfer in complexes Cp2MCl2 (Cp=Ï€-C5H5, M=Ti,) Tj ETQq0 0 0 rgBT /Overlock 1	1.8	21

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91	A theoretical study on the cyclopropane adsorption onto the copper surfaces by density functional theory and quantum chemical molecular dynamics methods. Journal of Molecular Catalysis A, 2004, 220, 189-198.	4.8	21
92	Chemical reaction dynamics of PeCB and TCDD decomposition: A tight-binding quantum chemical molecular dynamics study with first-principles parameterization. International Journal of Quantum Chemistry, 2005, 102, 318-327.	2.0	21
93	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
94	Reactive Molecular Dynamics Simulations of Wear and Tribochemical Reactions of Diamond like Carbon Interfaces with Nanoscale Asperities under H2 Gas: Implications for Solid Lubricant Coatings. ACS Applied Nano Materials, 2020, 3, 7297-7304.	5.0	21
95	Nonâ€Empirical Law for Nanoscale Atomâ€byâ€Atom Wear. Advanced Science, 2021, 8, 2002827.	11.2	21
96	Tight-binding quantum chemical molecular dynamics study of cathode materials for lithium secondary battery. Solid State Ionics, 2002, 152-153, 273-277.	2.7	20
97	Adsorption of NH 3 , NO 2 and NO on copper-aluminate catalyst: an ab initio density functional study. Theoretical Chemistry Accounts, 2003, 109, 190-194.	1.4	20
98	Quantum Chemical Molecular Dynamics Studies on the Chemical Mechanical Polishing Process of Cu Surface. Japanese Journal of Applied Physics, 2003, 42, 1897-1902.	1.5	20
99	Parallel Large-Scale Molecular Dynamics Simulation Opens New Perspective to Clarify the Effect of a Porous Structure on the Sintering Process of Ni/YSZ Multiparticles. ACS Applied Materials & Interfaces, 2017, 9, 31816-31824.	8.0	20
100	Simulation of Atomic Force Microscopy Image Variations along the Surface Normal: Presence of Possible Resolution Limit in the Attractive Force Range. Japanese Journal of Applied Physics, 1995, 34, L789-L792.	1.5	19
101	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
102	A theoretical investigation on the abrasive wear prevention mechanism of ZDDP and ZP tribofilms. Applied Surface Science, 2008, 254, 7976-7979.	6.1	19
103	Tribochemical Degradation of Polytetrafluoroethylene Catalyzed by Copper and Aluminum Surfaces. Journal of Physical Chemistry C, 2016, 120, 10857-10865.	3.1	19
104	First-Principles Molecular Dynamics Study of Silicon-Based Ceramics: Different Tribochemical Reaction Mechanisms during the Running-in Period of Silicon Nitride and Silicon Carbide. Journal of Physical Chemistry C, 2020, 124, 20079-20089.	3.1	19
105	Atom-by-Atom and Sheet-by-Sheet Chemical Mechanical Polishing of Diamond Assisted by OH Radicals: A Tight-Binding Quantum Chemical Molecular Dynamics Simulation Study. ACS Applied Materials & Interfaces, 2021, 13, 41231-41237.	8.0	19
106	Atomic processes in the deposition and sintering of ultrafine metal particles on MgO(001) as investigated by molecular dynamics and computer graphics. Applied Surface Science, 1994, 75, 51-57.	6.1	18
107	Combinatorial computational chemistry approach to the design of methanol synthesis catalyst. Applied Surface Science, 2002, 189, 253-259.	6.1	18
108	Density functional theory and tight-binding quantum chemical molecular dynamics calculations on Ce1â€“xCuxO2â€“Î´ catalyst and the adsorptions of CH3OH and CH3O on Ce1â€“xCuxO2â€“Î´. Chemical Physics Letters, 2004, 384, 30-34.	2.6	18

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109	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
110	COMPUTATIONAL CHEMISTRY FOR INDUSTRIAL INNOVATION. Reviews in Chemical Engineering, 2006, 22, .	4.4	18
111	Adsorption and dissociation of molecular hydrogen on Pt/CeO2 catalyst in the hydrogen spillover process: A quantum chemical molecular dynamics study. Applied Surface Science, 2010, 256, 7643-7652.	6.1	18
112	Communication: Different behavior of Young's modulus and fracture strength of CeO2: Density functional theory calculations. Journal of Chemical Physics, 2014, 140, 121102.	3.0	18
113	Multi-nanoparticle model simulations of the porosity effect on sintering processes in Ni/YSZ and Ni/ScSZ by the molecular dynamics method. Journal of Materials Chemistry A, 2015, 3, 21518-21527.	10.3	18
114	Coarse-grained molecular dynamics simulation of the void growth process in the block structure of semicrystalline polymers. Modelling and Simulation in Materials Science and Engineering, 2016, 24, 055006.	2.0	18
115	Adsorption of NO on rhodium and palladium clusters: a density functional study. Applied Surface Science, 1997, 119, 318-320.	6.1	17
116	Adsorption of water vapor on the AlPO4-based catalysts and reaction mechanism for CFCs decomposition. Applied Catalysis A: General, 2004, 271, 55-60.	4.3	17
117	Modeling of Dye-Sensitized Solar Cells Based on TiO₂ Electrode Structure Model. Japanese Journal of Applied Physics, 2010, 49, 04DP10.	1.5	17
118	Multiscale Simulation of Electro-Chemo-Mechanical Coupling Behavior of PEN Structure under SOFC Operation. ECS Transactions, 2011, 35, 923-933.	0.5	17
119	Structures and Dynamics of Alkali Ion-exchanged ZSM-5 as Investigated by Molecular Dynamics and Computer Graphics. Chemistry Letters, 1991, 20, 2055-2058.	1.3	16
120	Density functional calculation on the adsorption of nitrogen oxides and water on ion exchanged ZSM-5. Applied Surface Science, 1998, 130-132, 561-565.	6.1	16
121	Possible Ferroelectricity in SnTiO3 by First-Principles Calculations. Materials Research Society Symposia Proceedings, 2002, 748, 1.	0.1	16
122	Density functional study of lanthanide complexes (Î·5-C5H5)2LnXÂ·OC4H8 (Ln=Laâ€“Lu; X=F, Cl, Br and I). Journal of Organometallic Chemistry, 2003, 679, 84-92.	1.8	16
123	Combinatorial computational chemistry approach to the design of metal catalysts for deNOx. Applied Surface Science, 2004, 223, 159-167.	6.1	16
124	Theoretical Calculations on Electronic Structure and Catalytic Reaction of Organo-f-element Complexes. Chemistry Letters, 2004, 33, 780-785.	1.3	16
125	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
126	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

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127	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
128	Experimental and Quantum Chemical Approaches to Develop Highly Selective Nanocatalysts for CO₂â€free Power Circulation. Chemical Record, 2016, 16, 2249-2259.	5.8	16
129	Different Etching Mechanisms of Diamond by Oxygen and Hydrogen Plasma: a Reactive Molecular Dynamics Study. Journal of Physical Chemistry C, 2021, 125, 16711-16718.	3.1	16
130	Application of Computer Graphics and Molecular Dynamics to the Investigation of Heterogeneous Catalysis.. Sekiyu Gakkaishi (Journal of the Japan Petroleum Institute), 1993, 36, 282-290.	0.1	16
131	Structure of TiO2 surfaces: a molecular dynamics study. Applied Surface Science, 1997, 119, 199-202.	6.1	15
132	Permeability of Ar and He through an inorganic membrane: a molecular dynamics study. Applied Surface Science, 1997, 119, 330-334.	6.1	15
133	Layer-by-layer heteroepitaxial growth process of a BaO layer on SrTiO3(001) as investigated by molecular dynamics. Journal of Chemical Physics, 1998, 109, 9148-9154.	3.0	15
134	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
135	The reason why thin-film silicon grows layer by layer in plasma-enhanced chemical vapor deposition. Scientific Reports, 2015, 5, 9052.	3.3	15
136	Molecular Dynamics Simulations of Chemically Disordered Ferroelectric (Ba,Sr)TiO₃ with a Semi-Empirical Effective Hamiltonian. Journal of the Physical Society of Japan, 2016, 85, 114714.	1.6	15
137	Cooperative roles of chemical reactions and mechanical friction in chemical mechanical polishing of gallium nitride assisted by OH radicals: tight-binding quantum chemical molecular dynamics simulations. Physical Chemistry Chemical Physics, 2021, 23, 4075-4084.	2.8	15
138	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
139	Molecular dynamics simulation of the friction between talc (001) surfaces. Applied Surface Science, 1997, 119, 335-340.	6.1	14
140	Independent and Interdependent Atomistic Structural Features of Pd Clusters Supported on the MgO(001) Surface. Journal of Physical Chemistry B, 1998, 102, 795-803.	2.6	14
141	Potential Energy Surface and Dynamics of Pd/MgO(001) System as Investigated by Periodic Density Functional Calculations and Classical Molecular Dynamics Simulations. Japanese Journal of Applied Physics, 2000, 39, 4255-4260.	1.5	14
142	Computational Chemistry Study on Crystal Growth of InGaN/GaN. Japanese Journal of Applied Physics, 2001, 40, 2991-2995.	1.5	14
143	Combinatorial computational chemistry approach to the design of cathode materials for a lithium secondary battery. Applied Surface Science, 2002, 189, 313-318.	6.1	14
144	Computational chemical study on separation of benzene and cyclohexane by a NaY zeolite membrane. Desalination, 2002, 147, 339-344.	8.2	14

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145	Photocatalytic oxidation dynamics of acetone on TiO2: tight-binding quantum chemical molecular dynamics study. Applied Surface Science, 2005, 244, 541-545.	6.1	14
146	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
147	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
148	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
149	Multi-scale theoretical study of support effect on sintering dynamics of Pt. Surface Science, 2009, 603, 3049-3056.	1.9	14
150	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
151	Polishing Process Simulation of SiO2 by CeO2 Abrasive Grain under Wet Environment. Hyomen Kagaku, 2012, 33, 351-356.	0.0	14
152	Simulation of Atomic Force Microscopy Images of Cleaved Mica Surfaces. Journal of Physical Chemistry B, 1997, 101, 4260-4264.	2.6	13
153	The Fate of a Cluster Colliding onto a Substrate Dissipation of Translational Kinetic Energy. Journal of Nanoparticle Research, 2001, 3, 213-218.	1.9	13
154	Density Functional Study of the Insertion and Ring-Opening Mechanism of MCP over Cp2LaH and Cp2LuH Catalysts. Journal of the American Chemical Society, 2003, 125, 16210-16212.	13.7	13
155	Development of Crystal Growth Simulator Based on Tight-Binding Quantum Chemical Molecular Dynamics Method and Its Application to Silicon Chemical Vapor Deposition Processes. Journal of Physical Chemistry C, 2012, 116, 12525-12531.	3.1	13
156	Different Crystal Growth Mechanisms of Si(001)-(2 Ã— 1):H during Plasma-Enhanced Chemical Vapor Deposition of SiH₃ and SiH₂ Radicals: Tight-Binding Quantum Chemical Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2013, 117, 15602-15614.	3.1	13
157	Tight-binding quantum chemical molecular dynamics simulations for the elucidation of chemical reaction dynamics in SiC etching with SF₆/O₂ plasma. Physical Chemistry Chemical Physics, 2016, 18, 7808-7819.	2.8	13
158	Molecular dynamics study of mesophase transitions upon annealing of imidazolium-based ionic liquids with long-alkyl chains. Physical Chemistry Chemical Physics, 2018, 20, 9796-9805.	2.8	13
159	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
160	Molecular Dynamics Simulations of Metal Clusters and Metal Deposition on Metal Surfaces. Japanese Journal of Applied Physics, 1995, 34, 6866-6872.	1.5	12
161	Simulation of AFM/LFM by molecular dynamics: role of lateral force in contact-mode AFM imaging. Surface Science, 1996, 357-358, 222-227.	1.9	12
162	Molecular dynamics simulation for ultrafine gold particles deposited on metal oxides. Catalysis Today, 1997, 36, 143-151.	4.4	12

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