Mauro Boero

List of Publications by Year in descending order

198 papers	6,322 citations	71061 41 h-index	79644 73 g-index
202 all docs	202 docs citations	202 times ranked	6223 citing authors

#	Article	IF	Citations
1	Thermal conductivity of amorphous SiO2 by first-principles molecular dynamics. Journal of Non-Crystalline Solids, 2022, 581, 121434.	1.5	10
2	Structural, dynamical, and electronic properties of the ionic liquid 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide. Physical Chemistry Chemical Physics, 2022, 24, 9597-9607.	1.3	3
3	Atomic structure of amorphous SiN: Combining Carâ€“Parrinello and Bornâ€“Oppenheimer first-principles molecular dynamics. Computational Materials Science, 2022, 211, 111555.	1.4	3
4	An atomistic insight into reactions and free-energy profiles of NH3 and Ga on GaN surfaces during the epitaxial growth. Applied Surface Science, 2022, 599, 153935.	3.1	1
5	How natural materials remove heavy metals from water: mechanistic insights from molecular dynamics simulations. Chemical Science, 2021, 12, 2979-2985.	3.7	7
6	First-principles thermal transport in amorphous Ge₂Sb₂Te₅ at the nanoscale. RSC Advances, 2021, 11, 10747-10752.	1.7	6
7	Estimation of the relative contributions to the electronic energy transfer rates based on FÃ¶rster theory: The case of C-phycocyanin chromophores. Biophysics and Physicobiology, 2021, 18, 196-214.	0.5	3
8	Quantitative assessment of the structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ge</mml:mi><mml:mn>20</mml:mn></mml:msub><mml:mathvariant="normal">I</mml:mi><mml:mn>7</mml:mn></mml:msub></mml:mrow></mml:math> chalcohalide glass by first-principles molecular dynamics. Physical Review B, 2021, 103, .	1.1	4
9	Tridentate complexes of group 4 bearing bis-aryloxide N-heterocyclic carbene ligand: Structure, spin density and charge states. Chemical Physics Letters, 2021, 781, 138888.	1.2	0
10	Chalcogenide glasses for innovation in applied science: fundamental issues and new insights. Journal Physics D: Applied Physics, 2020, 53, 033002.	1.3	4
11	Thermal resistance of an interfacial molecular layer by first-principles molecular dynamics. Journal of Chemical Physics, 2020, 153, 074704.	1.2	7
12	Atomic Structure of Glassy GeTe₄ as a Playground to Assess the Performances of Density Functional Schemes Accounting for Dispersion Forces. Journal of Physical Chemistry B, 2020, 124, 11273-11279.	1.2	7
13	A two-dimensional liquid-like phase on Ga-rich GaN (0001) surfaces evidenced by first principles molecular dynamics. Japanese Journal of Applied Physics, 2020, 59, SGGK04.	0.8	5
14	Heat transport in disordered network forming materials: Size effects and existence of propagative modes. Computational Materials Science, 2020, 177, 109607.	1.4	4
15	Making Computer Materials Real: The Predictive Power of First-Principles Molecular Dynamics. Springer Series in Materials Science, 2020, , 3-21.	0.4	1
16	Reaction mechanism of N-cyclopropylglycine oxidation by monomeric sarcosine oxidase. Physical Chemistry Chemical Physics, 2020, 22, 16552-16561.	1.3	4
17	Unique protonation states of aspartate and topaquinone in the active site of copper amine oxidase. RSC Advances, 2020, 10, 38631-38639.	1.7	8
18	Atomic structure and origin of chirality of DNA-stabilized silver clusters. Physical Review Materials, 2020, 4, .	0.9	13

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19	Role of the Propionic Acid Side-Chain of C-Phycocyanin Chromophores in the Excited States for the Photosynthesis Process. Bulletin of the Chemical Society of Japan, 2020, 93, 1509-1519.	2.0	8
20	Assessing the Versatility of Molecular Modelling as a Strategy for Predicting Gas Adsorption Properties of Chalcogels. Springer Series in Materials Science, 2020, , 23-37.	0.4	0
21	Computics Approach toward Clarification of Atomic Reactions during Epitaxial Growth of GaN. , 2020, , .		1
22	Unique Structural Relaxations and Molecular Conformations of Porphyra-334 at the Excited State. Journal of Physical Chemistry B, 2019, 123, 7649-7656.	1.2	13
23	Chalcogenide glasses as a playground for the application of first-principles molecular dynamics to disordered materials. Solid State Sciences, 2019, 95, 105925.	1.5	4
24	Molecular attachment to a microscope tip: inelastic tunneling, Kondo screening, and thermopower. Beilstein Journal of Nanotechnology, 2019, 10, 1243-1250.	1.5	1
25	Hydrogen storage mechanism and diffusion in metalâ€“organic frameworks. Physical Chemistry Chemical Physics, 2019, 21, 7756-7764.	1.3	35
26	High Turnover Frequency COâ€“NO Reactions over Rh Overlayer Catalysts: A Comparative Study Using Rh Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 6080-6089.	1.5	26
27	Screening the 4f-electron spin of TbPc₂ single-molecule magnets on metal substrates by ligand channeling. Nanoscale, 2019, 11, 21167-21179.	2.8	17
28	Thermal conductivity and transport modes in glassy <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>GeTe</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math> by first-principles molecular dynamics. Physical Review Materials, 2019, 3, .	0.9	11
29	First-principles study of the atomic structure of glassy Ga10Ge15Te75. Journal of Non-Crystalline Solids, 2018, 498, 338-344.	1.5	8
30	Synthesis and Characterization of Non-Isolated-Pentagon-Rule Actinide Endohedral Metallofullerenes U@C₁(17418)-C₇₆, U@C₁(28324)-C₈₀, and Th@C₁(28324)-C₈₀: Low-Symmetry Cage Selection Directed by a Tetravalent Ion. Journal of the American Chemical Society, 2018, 140, 18039-18050.	6.6	73
31	Sensitivity to Dispersion Forces in First-Principles Modeling of Disordered Chalcogenides. Frontiers in Materials, 2018, 5, .	1.2	7
32	A detailed insight into the catalytic reduction of NO operated by Crâ€“Cu nanostructures embedded in a CeO₂ surface. Physical Chemistry Chemical Physics, 2018, 20, 25592-25601.	1.3	14
33	On the occurrence of size effects in the calculation of thermal conductivity by first-principles molecular dynamics: The case of glassy GeTe4. Journal of Non-Crystalline Solids, 2018, 498, 190-193.	1.5	13
34	The structure and dipolar properties of CO2 adsorbed in a porous glassy chalcogel: Insights from first-principles molecular dynamics. Journal of Non-Crystalline Solids, 2018, 498, 288-293.	1.5	4
35	The role of dispersion forces on the atomic structure of glassy chalcogenides: The case of GeSe4 and GeS4. Journal of Non-Crystalline Solids, 2018, 499, 167-172.	1.5	8
36	Evaluating the Critical Roles of Precursor Nature and Water Content When Tailoring Magnetic Nanoparticles for Specific Applications. ACS Applied Nano Materials, 2018, 1, 4306-4316.	2.4	22

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37	First-Principles Study of Dissociation Processes for the Synthesis of Fe and Co Oxide Nanoparticles. Journal of Chemical Theory and Computation, 2018, 14, 225-235.	2.3	6
38	Microscopic Mechanisms of Initial Formation Process of Graphene on SiC(0001) Surfaces: Selective Si Desorption from Step Edges. Journal of Physical Chemistry C, 2017, 121, 5041-5049.	1.5	8
39	How seaweeds release the excess energy from sunlight to surrounding sea water. Physical Chemistry Chemical Physics, 2017, 19, 15745-15753.	1.3	17
40	Thermal conductivity of glassy GeTe₄by first-principles molecular dynamics. Physical Chemistry Chemical Physics, 2017, 19, 9729-9732.	1.3	30
41	First-Principles Calculations That Clarify Energetics and Reactions of Oxygen Adsorption and Carbon Desorption on 4H-SiC (112ì...0) Surface. Journal of Physical Chemistry C, 2017, 121, 3920-3928.	1.5	8
42	An atomic-level insight into the basic mechanism responsible for the enhancement of the catalytic oxidation of carbon monoxide on a Cu/CeO₂ surface. Physical Chemistry Chemical Physics, 2017, 19, 3498-3505.	1.3	6
43	Role of Ï€-Radicals in the Spin Connectivity of Clusters and Networks of Tb Double-Decker Single Molecule Magnets. ACS Nano, 2017, 11, 10750-10760.	7.3	24
44	Indirect Four-Electron Oxygen Reduction Reaction on Carbon Materials Catalysts in Acidic Solutions. ACS Catalysis, 2017, 7, 7908-7916.	5.5	42
45	Layered Simple Hydroxides Functionalized by Fluoreneâ€Phosphonic Acids: Synthesis, Interface Theoretical Insights, and Magnetoelectric Effect. Advanced Functional Materials, 2017, 27, 1703576.	7.8	20
46	Impact of dispersion forces on the atomic structure of a prototypical network-forming disordered system: The case of liquid GeSe2. Journal of Chemical Physics, 2017, 147, 044504.	1.2	9
47	Simple but Efficient Method for Inhibiting Sintering and Aggregation of Catalytic Pt Nanoclusters on Metalâ€Oxide Supports. Chemistry - A European Journal, 2017, 23, 1531-1538.	1.7	7
48	Atomic-scale structure of the glassy <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ge</mml:mi><mml:mn>2</mml:mn></mml: phase change material: A quantitative assessment via first-principles molecular dynamics. Physical Review B, 2017, 96, .	1.1	24
49	The role of 2D/3D spin-polarization interactions in hybrid copper hydroxide acetate: new insights from first-principles molecular dynamics. Beilstein Journal of Nanotechnology, 2017, 8, 857-860.	1.5	4
50	The absence of a gap state and enhancement of the Marsâ€“van Krevelen reaction on oxygen defective Cu/CeO2 surfaces. Physical Chemistry Chemical Physics, 2016, 18, 20708-20712.	1.3	4
51	Pressure-induced structural changes in the network-forming isostatic glass<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>GeSe</mml:mi><mml:mn>4</mml:mn></mml:msub></ An investigation by neutron diffraction and first-principles molecular dynamics. Physical Review B, 2016, 93, .	1.1	24
52	Reducing the Cost and Preserving the Reactivity in Nobleâ€Metalâ€Based Catalysts: Oxidation of CO by Pt and Alâ€“Pt Alloy Clusters Supported on Graphene. Chemistry - A European Journal, 2016, 22, 5181-5188.	1.7	14
53	Stability and Destabilization Processes in the Formation of Ferrocene-Based Metalâ€“Organic Moleculeâ€“Metal Nano-Junctions. Journal of Physical Chemistry C, 2016, 120, 13825-13830.	1.5	8
54	Carâ€“Parrinello Molecular Dynamics. , 2016, , 489-497.		0

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55	Role of the van der Waals interactions and impact of the exchange-correlation functional in determining the structure of glassyGeTe4. Physical Review B, 2015, 92, .	1.1	43
56	Theoretical design of a novel copper doped gold cluster supported on graphene utilizing ab initio molecular dynamics simulations. AIP Conference Proceedings, 2015, , .	0.3	0
57	Role of van der Waals corrections in first principles simulations of alkali metal ions in aqueous solutions. Journal of Chemical Physics, 2015, 143, 194510.	1.2	30
58	Exohedral Mâ€“C60 and M2â€“C60 (M = Pt, Pd) systems as tunable-gap building blocks for nanoarchitecture and nanocatalysis. Journal of Chemical Physics, 2015, 143, 114308.	1.2	6
59	Carâ€“Parrinello Molecular Dynamics. , 2015, , 1-10.		2
60	Reaction Pathway and Free Energy Landscape of Catalytic Oxidation of Carbon Monoxide Operated by a Novel Supported Goldâ€“Copper Alloy Cluster. Journal of Physical Chemistry C, 2015, 119, 15421-15427.	1.5	8
61	First-principles study of amorphous<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ga</mml:mi><mml:mn>1.4</mml:mn></mml:msub></mml:mrow></mml:math>alloys. Physical Review B, 2015, 91, .	1.1	21
62	Origin of structural analogies and differences between the atomic structures of GeSe4 and GeS4 glasses: A first principles study. Journal of Chemical Physics, 2015, 143, 034504.	1.2	35
63	Unraveling the degradation of artificial amide bonds in nylon oligomer hydrolase: from induced-fit to acylation processes. Physical Chemistry Chemical Physics, 2015, 17, 4492-4504.	1.3	12
64	First-Principles Modeling of Binary Chalcogenides: Recent Accomplishments and New Achievements. Springer Series in Materials Science, 2015, , 313-344.	0.4	3
65	Density-driven defect-mediated network collapse of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">GeSe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>glass. Physical Review B, 2014, 90, .	1.1	30
66	Surface of glassyGeS2: A model based on a first-principles approach. Physical Review B, 2014, 90, .	1.1	16
67	Metalâ€“organic moleculeâ€“metal nano-junctions: a close contact between first-principles simulations and experiments. Journal of Physics Condensed Matter, 2014, 26, 104206.	0.7	7
68	Nylon-Oligomer Hydrolase Promoting Cleavage Reactions in Unnatural Amide Compounds. Journal of Physical Chemistry Letters, 2014, 5, 1210-1216.	2.1	13
69	Tuning Magnetic Properties with Pressure in Hybrid Organicâ€“Inorganic Materials: The Case of Copper Hydroxide Acetate. Journal of Physical Chemistry C, 2014, 118, 18700-18705.	1.5	7
70	The Role of Ni-Based Cocatalyst in Inhomogeneous RVO₄ Photocatalyst Systems (R = Y, Gd). Journal of Physical Chemistry C, 2014, 118, 12845-12854.	1.5	13
71	Steric and electronic selectivity in the synthesis of Fe-1,2,4,5-tetracyanobenzene (TCNB) complexes on Au(111): From topological confinement to bond formation. Nano Research, 2014, 7, 888-897.	5.8	24
72	Inhomogeneous RVO₄ Photocatalyst Systems (R = Y, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er,) Tj ETQq0 0 0 rgBT /Overlock 10	1.5	47

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73	Structure, topology, rings, and vibrational and electronic properties of Ge<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>Se<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>glasses across the rigidity transition: A numerical study. Physical Review B, 2013, 88, .	1.1	76
74	Stability of Ge12C48 and Ge20C40 heterofullerenes: A first principles molecular dynamics study. Chemical Physics Letters, 2013, 556, 163-167.	1.2	4
75	Compositional Thresholds and Anomalies in Connection with Stiffness Transitions in Network Glasses. Physical Review Letters, 2013, 110, 165501.	2.9	61
76	Atom-Scale Reaction Pathways and Free-Energy Landscapes in Oxygen Plasma Etching of Graphene. Journal of Physical Chemistry Letters, 2013, 4, 1592-1596.	2.1	31
77	The structure of liquid GeSe revisited: A first principles molecular dynamics study. Journal of Chemical Physics, 2013, 138, 174505.	1.2	21
78	Formation of a Covalent Glycosylâ€“Enzyme Species in a Retaining Glycosyltransferase. Chemistry - A European Journal, 2013, 19, 14018-14023.	1.7	50
79	First-principles molecular dynamics study of glassy GeS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>: Atomic structure and bonding properties. Physical Review B, 2013, 88, .	1.1	33
80	Communication: Hydration structure and polarization of heavy alkali ions: A first principles molecular dynamics study of Rb+ and Cs+. Journal of Chemical Physics, 2012, 137, 041101.	1.2	30
81	First principles investigation of the atomic structure and magnetic properties of copper hydroxide acetate. Comptes Rendus Chimie, 2012, 15, 202-208.	0.2	5
82	Structural properties of glassy Ge<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Se<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>from first-principles molecular dynamics. Physical Review B, 2012, 86, .	1.1	33
83	Microscopic mechanisms of initial oxidation of Si(100): Reaction pathways and free-energy barriers. Physical Review B, 2012, 85, .	1.1	15
84	Tautomers of extended reduced pyrazinacenes: a density-functional-theory based study. Physical Chemistry Chemical Physics, 2011, 13, 2145-2150.	1.3	9
85	LeuRS Synthetase: A First-Principles Investigation of the Water-Mediated Editing Reaction. Journal of Physical Chemistry B, 2011, 115, 12276-12286.	1.2	20
86	Effect of Hydrogen Termination on Carbon K-Edge X-ray Absorption Spectra of Nanographene. Journal of Physical Chemistry C, 2011, 115, 5392-5403.	1.5	44
87	The initiation mechanisms for surface hydrosilylation with 1-alkenes. Physical Chemistry Chemical Physics, 2011, 13, 4862.	1.3	14
88	Self-diffusion in crystalline silicon: A Car-Parrinello molecular dynamics study. Physical Review B, 2011, 84, .	1.1	9
89	Interacting Lewis-X Carbohydrates in Condensed Phase: A First-Principles Molecular Dynamics Study. Journal of Physical Chemistry B, 2011, 115, 12599-12606.	1.2	2
90	Structural properties of liquid Ge<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Se<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>: A first-principles study. Physical Review B, 2011, 84, .	1.1	22

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91	Thermal behavior of Si-doped fullerenes vs their structural stability at T=0K: A density functional study. Chemical Physics Letters, 2011, 510, 14-17.	1.2	17
92	Selective nitrogen doping in graphene: Enhanced catalytic activity for the oxygen reduction reaction. Physical Review B, 2011, 84, .	1.1	33
93	Angular rigidity in tetrahedral network glasses with changing composition. Physical Review B, 2011, 84, .	1.1	79
94	Dispersion and Localization of Electronic States at a Ferrocene/Cu(111) Interface. Physical Review Letters, 2011, 107, 216801.	2.9	55
95	From Salicylaldehyde to Chiral Salen Sulfonates - Syntheses, Structures and Properties of New Transition Metal Complexes Derived from Sulfonato Salen Ligands. European Journal of Inorganic Chemistry, 2010, 2010, 4450-4461.	1.0	22
96	Electronic structure and localization properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>C</mml:mtext><mml:mrow><mml:mn>60</mml:mn></mml:mrow></mml:msu xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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109	A Mechanism of Adsorption of Î²â€Nicotinamide Adenine Dinucleotide on Graphene Sheets: Experiment and Theory. Chemistry - A European Journal, 2009, 15, 10851-10856.	1.7	105
110	Water molecule adsorption properties on surfaces of MVO4 (M = In, Y, Bi) photo-catalysts. Journal of Electroceramics, 2009, 22, 114-119.	0.8	21
111	Hydrogenation of ultrasmall carbon nanotubes: A first principle study. Chemical Physics Letters, 2009, 480, 215-219.	1.2	10
112	Ab-initio molecular dynamical study of a single transition metal atom on fullerene C60: the case of Ta. European Physical Journal D, 2009, 51, 369-374.	0.6	2
113	Conformational Changes in a Flexible, Encapsulated Dicarboxylate: Evidence from Density Functional Theory Simulations. Journal of Physical Chemistry A, 2009, 113, 9075-9079.	1.1	4
114	Water Solvation Properties: An Experimental and Theoretical Investigation of Salt Solutions at Finite Dilution. Journal of Physical Chemistry A, 2009, 113, 7725-7729.	1.1	26
115	First-principles calculation of the electronic properties of graphene clusters doped with nitrogen and boron: Analysis of catalytic activity for the oxygen reduction reaction. Physical Review B, 2009, 80, .	1.1	177
116	Evidence for a ball-shaped cyclen cyclophane: an experimental and first principles study. Physical Chemistry Chemical Physics, 2009, 11, 6038.	1.3	12
117	1P-105 Computational analysis of electronic structures of hemes a / a_3 of the bovine cytochrome c oxidase in the reduced and oxidized states(Electronic state, The 47th Annual Meeting of the) Tj ETQq1 1 0.784314 rgBT /Overlock 10	0.0	0
118	A First-Principle Exploration of Heme <I>a</I> and Heme <I>a</I>₃ of the Bovine Cytochrome <I>c</I> Oxidase in Reduced and Oxidized Charge States. Journal of Computational and Theoretical Nanoscience, 2009, 6, 2640-2647.	0.4	2
119	Dissociation of water molecule at three-fold oxygen coordinated V site on the InVO4 (001) surface. Applied Surface Science, 2008, 255, 679-681.	3.1	7
120	Carbon Alloy Catalysts: Active Sites for Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2008, 112, 14706-14709.	1.5	474
121	Enzymatic Reaction Mechanisms of RNA Enzyme (Ribozyme) Revealed by First Principles Molecular Dynamics Simulations. Seibutsu Butsuri, 2008, 48, 216-220.	0.0	0
122	Charge localisation and hopping in DNA. Molecular Simulation, 2007, 33, 57-60.	0.9	9
123	First principles molecular dynamics study of catalytic reactions of biological macromolecular systems: toward analyses with QM/MM hybrid molecular simulations. Journal of Physics Condensed Matter, 2007, 19, 365217.	0.7	4
124	First-principles molecular dynamics study of proton transfer mechanism in bovine cytochromecoxidase. Journal of Physics Condensed Matter, 2007, 19, 365220.	0.7	8
125	Hydration of alkali ions from first principles molecular dynamics revisited. Journal of Chemical Physics, 2007, 126, 034501.	1.2	147
126	Role of Nitrogen Atoms in Reduction of Electron Charge Traps in Hf-Based High- $kappa$ Dielectrics. IEEE Electron Device Letters, 2007, 28, 363-365.	2.2	19

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127	Excess Electron in Water at Different Thermodynamic Conditions. Journal of Physical Chemistry A, 2007, 111, 12248-12256.	1.1	58
128	Possible Mechanism of Proton Transfer through Peptide Groups in the H-Pathway of the Bovine Cytochrome c Oxidase. Journal of the American Chemical Society, 2007, 129, 9663-9673.	6.6	61
129	Hydration properties of magnesium and calcium ions from constrained first principles molecular dynamics. Journal of Chemical Physics, 2007, 127, 074503.	1.2	141
130	Water Molecule Adsorption Properties on the BiVO4(100) Surface. Journal of Physical Chemistry B, 2006, 110, 9188-9194.	1.2	68
131	Hsc70 ATPase:Â An Insight into Water Dissociation and Joint Catalytic Role of K+and Mg2+Metal Cations in the Hydrolysis Reaction. Journal of the American Chemical Society, 2006, 128, 16798-16807.	6.6	59
132	Enol-to-keto Tautomerism of Peptide Groups. Journal of Physical Chemistry B, 2006, 110, 4443-4450.	1.2	24
133	1P182 Theoretical Investigation into Proton Transfer Mechanism Involving Peptide Bonds(5. Heme) Tj ETQq1 1 0.784314 rgBT /Overlo S192.	0.0	0
134	First-principle molecular dynamics study of bond disruption and formation in SiO2 upon irradiation. Physica B: Condensed Matter, 2006, 376-377, 945-949.	1.3	3
135	Unique behavior of F-centers in high-k Hf-based oxides. Physica B: Condensed Matter, 2006, 376-377, 392-394.	1.3	13
136	Double Proton Coupled Charge Transfer in DNA. Angewandte Chemie - International Edition, 2006, 45, 5606-5609.	7.2	52
137	Asymmetric Distribution of Charge Trap in HfO2-Based High-k Gate Dielectrics. ECS Transactions, 2006, 1, 777-788.	0.3	0
138	Extensive Studies for Effects of Nitrogen Incorporation into Hf-based High-k Gate Dielectrics. ECS Transactions, 2006, 2, 63-78.	0.3	1
139	Structural, electronic, and optical properties of the diindenoperylene molecule from first-principles density-functional theory. Physical Review A, 2006, 74, .	1.0	23
140	Water Molecule Adsorption Properties and Electronic Structures of Metal Oxide Photo-catalysts Designed for Water Decomposition. , 2006, , .		1
141	Free energy molecular dynamics simulations of pulsed-laser-irradiated SiO2: Siâ€“Si bond formation in a matrix of SiO2. Applied Physics Letters, 2005, 86, 201910.	1.5	18
142	Hydrophobic-Hydrophilic Interactions of Water with Alkanethiolate Chains from First-Principles Calculations. ChemPhysChem, 2005, 6, 1889-1893.	1.0	5
143	Density and Temperature Dependence of Proton Diffusion in Water: A First-Principles Molecular Dynamics Study. ChemPhysChem, 2005, 6, 1775-1779.	1.0	52
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145	Double-Metal-Ion/Single-Metal-Ion Mechanisms of the Cleavage Reaction of Ribozymes:Â First-Principles Molecular Dynamics Simulations of a Fully Hydrated Model System. Journal of Chemical Theory and Computation, 2005, 1, 925-934.	2.3	47
146	Tantalum-fullerene clusters:â€ƒA first-principles study of static properties and dynamical behavior. Physical Review B, 2004, 70, .	1.1	16
147	E' CENTERS IN SILICON DIOXIDE: FIRST-PRINCIPLES MOLECULAR DYNAMICS STUDIES. Modern Physics Letters B, 2004, 18, 707-724.	1.0	13
148	Hydrogen Bond Driven Chemical Reactions:Â Beckmann Rearrangement of Cyclohexanone Oxime into Îµ-Caprolactam in Supercritical Water. Journal of the American Chemical Society, 2004, 126, 6280-6286.	6.6	125
149	A Possible Origin of Carrier Doping into DNA. Journal of the Physical Society of Japan, 2004, 73, 2089-2092.	0.7	26
150	The electronic structures of the thin films of InVO4 and TiO2 by first principles calculations. Thin Solid Films, 2003, 445, 168-174.	0.8	30
151	First-Principles Molecular-Dynamics Simulations of a Hydrated Electron in Normal and Supercritical Water. Physical Review Letters, 2003, 90, 226403.	2.9	156
152	Eâ€²Centers inÎ±Quartz in the Absence of Oxygen Vacancies: A First-Principles Molecular-Dynamics Study. Physical Review Letters, 2003, 91, 206401.	2.9	27
153	Carâ€”Parrinello study of Zieglerâ€”Natta heterogeneous catalysis: stability and destabilization problems of the active site models. Molecular Physics, 2002, 100, 2935-2940.	0.8	29
154	Adsorption of water molecules on the surface of photo-catalyst: a first principles theoretical comparison between InVO₄ and rutile TiO₂. Materials Research Society Symposia Proceedings, 2002, 751, 1.	0.1	1
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