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	Carbon Alloy Catalysts: Active Sites for Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2008, 112, 14706-14709.	1.5	474
2	Alq3: ab initio calculations of its structural and electronic properties in neutral and charged states. Chemical Physics Letters, 1998, 294, 263-271.	1.2	350
3	Electronic structures of promising photocatalysts InMO4 (M=V, Nb, Ta) and BiVO4 for water decomposition in the visible wavelength region. Journal of Chemical Physics, 2002, 117, 7313-7318.	1.2	231
4	First Principles Molecular Dynamics Study of Zieglerâ^'Natta Heterogeneous Catalysis. Journal of the American Chemical Society, 1998, 120, 2746-2752.	6.6	229
5	Structure and Hyperfine Parameters ofE1â€²Centers inÎ±-Quartz and in VitreousSiO2. Physical Review Letters, 1997, 78, 887-890.	2.9	207
6	First Principles Study of Propene Polymerization in Zieglerâ^'Natta Heterogeneous Catalysis. Journal of the American Chemical Society, 2000, 122, 501-509.	6.6	198
7	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
8	First-Principles Molecular-Dynamics Simulations of a Hydrated Electron in Normal and Supercritical Water. Physical Review Letters, 2003, 90, 226403.	2.9	156
9	Hydrogen Bonding and Dipole Moment of Water at Supercritical Conditions: A First-Principles Molecular Dynamics Study. Physical Review Letters, 2000, 85, 3245-3248.	2.9	151
10	Hydration of alkali ions from first principles molecular dynamics revisited. Journal of Chemical Physics, 2007, 126, 034501.	1.2	147
11	Hydration properties of magnesium and calcium ions from constrained first principles molecular dynamics. Journal of Chemical Physics, 2007, 127, 074503.	1.2	141
12	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
13	A First Principles Exploration of a Variety of Active Surfaces and Catalytic Sites in Zieglerâ^'Natta Heterogeneous Catalysis. Journal of Physical Chemistry A, 2001, 105, 5096-5105.	1.1	123
14	Water at supercritical conditions: A first principles study. Journal of Chemical Physics, 2001, 115, 2219-2227.	1.2	123
15	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
16	Influence of hydrogen-bonding configurations on the physical properties of hydrogenated amorphous silicon. Physical Review B, 1994, 50, 18046-18053.	1.1	97
17	First principles calculations of Si doped fullerenes: Structural and electronic localization properties in C59Si and C58Si2. Journal of Chemical Physics, 1999, 111, 6787-6796.	1.2	90
18	Angular rigidity in tetrahedral network glasses with changing composition. Physical Review B, 2011, 84, .	1.1	79

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19	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>glasse	1.1	76
20	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
21	Enhanced Catalytic Activity of Carbon Alloy Catalysts Codoped with Boron and Nitrogen for Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2010, 114, 8933-8937.	1.5	70
22	Water Molecule Adsorption Properties on the BiVO4(100) Surface. Journal of Physical Chemistry B, 2006, 110, 9188-9194.	1.2	68
23	Ab InitioSimulations of Photoinduced Interconversions of Oxygen Deficient Centers in Amorphous Silica. Physical Review Letters, 2001, 87, 195504.	2.9	63
24	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
25	Compositional Thresholds and Anomalies in Connection with Stiffness Transitions in Network Glasses. Physical Review Letters, 2013, 110, 165501.	2.9	61
26	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
27	Excess Electron in Water at Different Thermodynamic Conditions. Journal of Physical Chemistry A, 2007, 111, 12248-12256.	1.1	58
28	Catalytic Role of Metal Ion in the Selection of Competing Reaction Paths:Â A First Principles Molecular Dynamics Study of the Enzymatic Reaction in Ribozyme. Journal of the American Chemical Society, 2002, 124, 8949-8957.	6.6	55
29	Dispersion and Localization of Electronic States at a Ferrocene/Cu(111) Interface. Physical Review Letters, 2011, 107, 216801.	2.9	55
30	Charge Localization in DNA Fibers. Physical Review Letters, 2005, 94, 158103.	2.9	53
31	Density and Temperature Dependence of Proton Diffusion in Water: A First-Principles Molecular Dynamics Study. ChemPhysChem, 2005, 6, 1775-1779.	1.0	52
32	Double Proton Coupled Charge Transfer in DNA. Angewandte Chemie - International Edition, 2006, 45, 5606-5609.	7.2	52
33	Ab initioSimulation of Phase Transitions and Dissociation ofH2Sat High Pressure. Physical Review Letters, 2000, 85, 1254-1257.	2.9	50
34	Formation of a Covalent Glycosylâ€“Enzyme Species in a Retaining Glycosyltransferase. Chemistry - A European Journal, 2013, 19, 14018-14023.	1.7	50
35	Experimental and computational studies of heterofullerenes. Scripta Materialia, 1999, 12, 1071-1076.	0.5	47
36	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

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37	Inhomogeneous RVO₄ Photocatalyst Systems (R = Y, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er,) Tj ETQq1 1 0.784314 rgBT /Ov	1.5	47
38	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
39	IBIC investigations on CVD diamond. Nuclear Instruments & Methods in Physics Research B, 1995, 100, 133-140.	0.6	43
40	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
41	A first principles investigation of water dipole moment in a defective continuous hydrogen bond network. Journal of Chemical Physics, 2009, 130, 024502.	1.2	42
42	Indirect Four-Electron Oxygen Reduction Reaction on Carbon Materials Catalysts in Acidic Solutions. ACS Catalysis, 2017, 7, 7908-7916.	5.5	42
43	Experimental and computational studies of Si-doped fullerenes. European Physical Journal D, 1999, 9, 337-340.	0.6	36
44	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
45	Hydrogen storage mechanism and diffusion in metalâ€“organic frameworks. Physical Chemistry Chemical Physics, 2019, 21, 7756-7764.	1.3	35
46	Grain size effects in CVD diamond detectors. Nuclear Instruments & Methods in Physics Research B, 1994, 93, 516-520.	0.6	33
47	Static Structure and Dynamical Correlations in High PressureH2S. Physical Review Letters, 1999, 83, 2218-2221.	2.9	33
48	Physical model of BTI, TDDB and SILC in W02-based high-k gate dielectrics. , 0, , .		33
49	Selective nitrogen doping in graphene: Enhanced catalytic activity for the oxygen reduction reaction. Physical Review B, 2011, 84, .	1.1	33
50	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
51	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
52	Zieglerâ€“Natta heterogeneous catalysis by first principles computer experiments. Surface Science, 1999, 438, 1-8.	0.8	31
53	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
54	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

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55	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
56	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
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	Thermal conductivity of glassy GeTe₄by first-principles molecular dynamics. Physical Chemistry Chemical Physics, 2017, 19, 9729-9732.	1.3	30
59	First principles calculations of iron-doped heterofullerenes. Computational Materials Science, 2000, 17, 191-195.	1.4	29
60	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
61	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
62	First principles study of thermal decomposition of alkylâ€“gallium and tertiary butylarsine. Journal of Chemical Physics, 2000, 112, 9549-9556.	1.2	26
63	A Possible Origin of Carrier Doping into DNA. Journal of the Physical Society of Japan, 2004, 73, 2089-2092.	0.7	26
64	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
65	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
66	Investigation of the Mechanism of Adsorption of Î²-Nicotinamide Adenine Dinucleotide on Single-Walled Carbon Nanotubes. Journal of Physical Chemistry Letters, 2010, 1, 122-125.	2.1	25
67	Enol-to-keto Tautomerism of Peptide Groups. Journal of Physical Chemistry B, 2006, 110, 4443-4450.	1.2	24
68	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
69	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></mml:math>: An investigation by neutron diffraction and first-principles molecular dynamics. Physical Review B, 2016, 93, .	1.1	24
70	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
71	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:msub></mml:mrow></mml:math> phase change material: A quantitative assessment via first-principles molecular dynamics. Physical Review B, 2017, 96, .	1.1	24
72	Structural, electronic, and optical properties of the diindenoperylene molecule from first-principles density-functional theory. Physical Review A, 2006, 74, .	1.0	23

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73	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
74	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
75	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
76	Water adsorption onto Y and V sites at the surface of the YVO4 photocatalyst and related electronic properties. Journal of Chemical Physics, 2009, 131, 034701.	1.2	21
77	Water molecule adsorption properties on surfaces of MVO4 (M = In, Y, Bi) photo-catalysts. Journal of Electroceramics, 2009, 22, 114-119.	0.8	21
78	The structure of liquid GeSe revisited: A first principles molecular dynamics study. Journal of Chemical Physics, 2013, 138, 174505.	1.2	21
79	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
80	LeuRS Synthetase: A First-Principles Investigation of the Water-Mediated Editing Reaction. Journal of Physical Chemistry B, 2011, 115, 12276-12286.	1.2	20
81	Layered Simple Hydroxides Functionalized by Fluoreneâ€Phosphonic Acids: Synthesis, Interface Theoretical Insights, and Magnetoelectric Effect. Advanced Functional Materials, 2017, 27, 1703576.	7.8	20
82	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
83	Car-parrinello molecular dynamics investigation of active surfaces and Ti catalytic sites in Ziegler-Natta heterogeneous catalysis. Macromolecular Symposia, 2001, 173, 137-148.	0.4	18
84	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
85	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
86	How seaweeds release the excess energy from sunlight to surrounding sea water. Physical Chemistry Chemical Physics, 2017, 19, 15745-15753.	1.3	17
87	Screening the 4f-electron spin of TbPc₂ single-molecule magnets on metal substrates by ligand channeling. Nanoscale, 2019, 11, 21167-21179.	2.8	17
88	Tantalum-fullerene clusters:â€ƒA first-principles study of static properties and dynamical behavior. Physical Review B, 2004, 70, .	1.1	16
89	Surface of glassyGeS2: A model based on a first-principles approach. Physical Review B, 2014, 90, .	1.1	16
90	Tautomerism in Reduced Pyrazinacenes. Journal of Chemical Theory and Computation, 2010, 6, 517-525.	2.3	15

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91	Microscopic mechanisms of initial oxidation of Si(100): Reaction pathways and free-energy barriers. Physical Review B, 2012, 85, .	1.1	15
92	Trimethylene isomers and propene: structural and vibrational properties from density functional theory. Chemical Physics Letters, 1997, 265, 24-34.	1.2	14
93	The initiation mechanisms for surface hydrosilylation with 1-alkenes. Physical Chemistry Chemical Physics, 2011, 13, 4862.	1.3	14
94	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
95	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
96	E' CENTERS IN SILICON DIOXIDE: FIRST-PRINCIPLES MOLECULAR DYNAMICS STUDIES. Modern Physics Letters B, 2004, 18, 707-724.	1.0	13
97	Unique behavior of F-centers in high-k Hf-based oxides. Physica B: Condensed Matter, 2006, 376-377, 392-394.	1.3	13
98	Nylon-Oligomer Hydrolase Promoting Cleavage Reactions in Unnatural Amide Compounds. Journal of Physical Chemistry Letters, 2014, 5, 1210-1216.	2.1	13
99	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
100	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
101	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
102	Atomic structure and origin of chirality of DNA-stabilized silver clusters. Physical Review Materials, 2020, 4, .	0.9	13
103	Evidence for a ball-shaped cyclen cyclophane: an experimental and first principles study. Physical Chemistry Chemical Physics, 2009, 11, 6038.	1.3	12
104	Protonation of a Hydroxide Anion Bridging Two Divalent Magnesium Cations in Water Probed by First-Principles Metadynamics Simulation. Journal of Physical Chemistry B, 2010, 114, 11102-11109.	1.2	12
105	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
106	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
107	Hydrogenation of ultrasmall carbon nanotubes: A first principle study. Chemical Physics Letters, 2009, 480, 215-219.	1.2	10
108	Thermal conductivity of amorphous SiO2 by first-principles molecular dynamics. Journal of Non-Crystalline Solids, 2022, 581, 121434.	1.5	10

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109	A novel VUV photochemical deposition apparatus. Applied Surface Science, 1993, 69, 127-132.	3.1	9
110	Charge localisation and hopping in DNA. Molecular Simulation, 2007, 33, 57-60.	0.9	9
111	Tautomers of extended reduced pyrazinacenes: a density-functional-theory based study. Physical Chemistry Chemical Physics, 2011, 13, 2145-2150.	1.3	9
112	Self-diffusion in crystalline silicon: A Car-Parrinello molecular dynamics study. Physical Review B, 2011, 84, .	1.1	9
113	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
114	Study of physical and chemical inhomogeneities in semiconducting and insulating materials by a combined use of micro-PIXE and micro-IBIC. Nuclear Instruments & Methods in Physics Research B, 1996, 109-110, 555-562.	0.6	8
115	First-principles molecular dynamics study of proton transfer mechanism in bovine cytochromecoxidase. Journal of Physics Condensed Matter, 2007, 19, 365220.	0.7	8
116	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
117	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
118	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
119	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
120	First-principles study of the atomic structure of glassy Ga10Ge15Te75. Journal of Non-Crystalline Solids, 2018, 498, 338-344.	1.5	8
121	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
122	Unique protonation states of aspartate and topaquinone in the active site of copper amine oxidase. RSC Advances, 2020, 10, 38631-38639.	1.7	8
123	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
124	Characterization of CVD diamond films by nuclear techniques with Î± particles. Diamond and Related Materials, 1995, 4, 517-519.	1.8	7
125	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
126	Energy Compensation Mechanism for Charge-Separated Protonation States in Aspartateâ˜Histidine Amino Acid Residue Pairs. Journal of Physical Chemistry B, 2010, 114, 6567-6578.	1.2	7

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127	Atomic Structure and Magnetic Nature of Copper Hydroxide Acetate. Journal of Physical Chemistry C, 2010, 114, 20213-20219.	1.5	7
128	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
129	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
130	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
131	Sensitivity to Dispersion Forces in First-Principles Modeling of Disordered Chalcogenides. Frontiers in Materials, 2018, 5, .	1.2	7
132	Thermal resistance of an interfacial molecular layer by first-principles molecular dynamics. Journal of Chemical Physics, 2020, 153, 074704.	1.2	7
133	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
134	How natural materials remove heavy metals from water: mechanistic insights from molecular dynamics simulations. Chemical Science, 2021, 12, 2979-2985.	3.7	7
135	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
136	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
137	First-principles thermal transport in amorphous Ge₂Sb₂Te₅ at the nanoscale. RSC Advances, 2021, 11, 10747-10752.	1.7	6
138	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
139	Hydrophobic-Hydrophilic Interactions of Water with Alkanethiolate Chains from First-Principles Calculations. ChemPhysChem, 2005, 6, 1889-1893.	1.0	5
140	First principles investigation of the atomic structure and magnetic properties of copper hydroxide acetate. Comptes Rendus Chimie, 2012, 15, 202-208.	0.2	5
141	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
142	Investigation on Microvoids in Pecvd a-Si:H. Materials Research Society Symposia Proceedings, 1993, 297, 231.	0.1	4
143	Car-Parrinello Simulation of Water at Supercritical Conditions. Progress of Theoretical Physics Supplement, 2000, 138, 259-261.	0.2	4
144	First Principles Molecular Dynamics Study of Catalysis for Polyolefins: the Ziegler-Natta Heterogeneous System.. International Journal of Molecular Sciences, 2002, 3, 395-406.	1.8	4

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145	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
146	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
147	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:m xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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