

# Stefano Baroni

## List of Articles by Year in descending order

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peer-reviewed  
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37359

52

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h-index

2993

194

g-index

209

documents

46503

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40022

55

h-index

50078

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#	ARTICLE	IF	CITATIONS
1	First-principles study of the gap in the spin excitation spectrum of the CrI <sub>3</sub> honeycomb ferromagnet. <i>Physical Review B</i> , 2023, 107, .	3.4	10
2	Magnon-phonon interactions enhance the gap at the Dirac point in the spin-wave spectra of CrI <sub>3</sub> two-dimensional magnets. <i>Physical Review B</i> , 2023, 107, .	3.4	26
3	Relationship between BDNF and oxytocin. <i>Comprehensive Psychoneuroendocrinology</i> , 2023, 16, 100207.	2.2	3
4	From borophene polymorphs towards a single honeycomb borophane phase: reduction of hexagonal boron layers on Al(111). <i>Nanoscale</i> , 2023, 15, 18407-18414.	5.0	4
5	Viscosity in water from first-principles and deep-neural-network simulations. <i>Npj Computational Materials</i> , 2022, 8, .	10.7	54
6	turboMagnon “A code for the simulation of spin-wave spectra using the Liouville-Lanczos approach to time-dependent density-functional perturbation theory. <i>Computer Physics Communications</i> , 2022, 280, 108500.	7.6	18
7	Growing borophene on metal substrates: A theoretical study of the role of oxygen on Al(111). <i>Physical Review Materials</i> , 2022, 6, .	2.7	5
8	Inflammatory and metabolic markers in patients with mood disorders. <i>World Journal of Biological Psychiatry</i> , 2021, 22, 228-235.	4.2	3
9	Cariprazine as a therapeutic option for schizophrenia: a drug evaluation. <i>Expert Opinion on Pharmacotherapy</i> , 2021, 22, 415-426.	2.1	5
10	Discovery of a natural cyan blue: A unique food-sourced anthocyanin could replace synthetic brilliant blue. <i>Science Advances</i> , 2021, 7, .	10.9	58
11	Decreased Plasma Oxytocin Levels in Patients With PTSD. <i>Frontiers in Psychology</i> , 2021, 12, .	2.2	30
12	Invariance principles in the theory and computation of transport coefficients. <i>European Physical Journal B</i> , 2021, 94, .	1.6	27
13	QEHeat: An open-source energy flux calculator for the computation of heat-transport coefficients from first principles. <i>Computer Physics Communications</i> , 2021, 269, 108090.	7.6	11
14	Thermal and Tidal Evolution of Uranus with a Growing Frozen Core. <i>Planetary Science Journal</i> , 2021, 2, 222.	3.9	31
15	Heat transport in liquid water from first-principles and deep neural network simulations. <i>Physical Review B</i> , 2021, 104, .	3.4	58
16	Heat and charge transport in H <sub>2</sub> O at ice-giant conditions from ab initio molecular dynamics simulations. <i>Nature Communications</i> , 2020, 11, .	13.7	31
17	Oxidation States, Thouless™ Pumps, and Nontrivial Ionic Transport in Nonstoichiometric Electrolytes. <i>Physical Review X</i> , 2020, 10, .	11.8	14
18	Electron energy loss spectroscopy of bulk gold with ultrasoft pseudopotentials and the Liouville-Lanczos method. <i>Physical Review B</i> , 2020, 102, .	3.4	19

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19	State-of-the-Art: Inflammatory and Metabolic Markers in Mood Disorders. <i>Life</i> , 2020, 10, 82.	2.7	18
20	Effectiveness of clozapine, oxcarbazepine and rivastigmine combination in a bipolar disorder patient with initial cerebral atrophy. <i>Clinical Case Reports (discontinued)</i> , 2020, 8, 254-257.	0.6	4
21	Title is missing!., 2020, .		7
22	Treatment of the obsessive-compulsive and bipolar disorders comorbidity: pharmacodynamic and pharmacokinetic evaluation. <i>Expert Opinion on Drug Metabolism and Toxicology</i> , 2019, 15, 619-631.	2.7	3
23	Topological quantization and gauge invariance of charge transport in liquid insulators. <i>Nature Physics</i> , 2019, 15, 967-972.	16.0	39
24	Modeling heat transport in crystals and glasses from a unified lattice-dynamical approach. <i>Nature Communications</i> , 2019, 10, .	13.7	233
25	Fast hybrid density-functional computations using plane-wave basis sets. <i>Electronic Structure</i> , 2019, 1, 015009.	2.5	43
26	Unraveling the molecular mechanisms of color expression in anthocyanins. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8757-8766.	2.7	34
27	Sex-Related Differences in Plasma Oxytocin Levels in Humans. <i>Clinical Practice and Epidemiology in Mental Health</i> , 2019, 15, 58-63.	2.0	71
28	Effect of Valproate and Antidepressant Drugs on Clozapine Metabolism in Patients With Psychotic Mood Disorders. <i>Therapeutic Drug Monitoring</i> , 2018, 40, 443-451.	1.8	13
29	Spin dynamics from time-dependent density functional perturbation theory. <i>European Physical Journal B</i> , 2018, 91, .	1.6	24
30	Ab initio study of electron energy loss spectra of bulk bismuth up to 100 eV. <i>Physical Review B</i> , 2017, 95, .	3.4	14
31	Accurate thermal conductivities from optimally short molecular dynamics simulations. <i>Scientific Reports</i> , 2017, 7, .	3.4	67
32	PM326. Internet addiction: an Italian study on university students. <i>International Journal of Neuropsychopharmacology</i> , 2016, 19, 16-16.	2.7	0
33	Asenapine augmentation in bipolar disorders: a case series. <i>Clinical Case Reports (discontinued)</i> , 2016, 4, 499-504.	0.6	4
34	Sampling Molecular Conformers in Solution with Quantum Mechanical Accuracy at a Nearly Molecular-Mechanics Cost. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4385-4389.	5.1	17
35	Multimodel Approach to the Optical Properties of Molecular Dyes in Solution. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4423-4429.	5.1	15
36	PT617. Plasma oxytocin levels in OCD patients. <i>International Journal of Neuropsychopharmacology</i> , 2016, 19, 26-26.	2.7	0

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37	Gauge Invariance of Thermal Transport Coefficients. <i>Journal of Low Temperature Physics</i> , 2016, 185, 79-86.	1.1	42
38	Current Trends on Antipsychotics: Focus on Asenapine. <i>Current Medicinal Chemistry</i> , 2016, 23, 2204-2216.	2.8	14
39	Ionizing radiation: brain effects and related neuropsychiatric manifestations. <i>Problemy Radiatsiinoi Medytsyny Ta Radiobiologii</i> , 2016, 21, 64-90.	0.4	11
40	turboEELSâ€”A code for the simulation of the electron energy loss and inelastic X-ray scattering spectra using the Liouvilleâ€”Lanczos approach to time-dependent density-functional perturbation theory. <i>Computer Physics Communications</i> , 2015, 196, 460-469.	7.6	78
41	Self-consistent continuum solvation for optical absorption of complex molecular systems in solution. <i>Journal of Chemical Physics</i> , 2015, 142, .	2.8	21
42	Accurate and Inexpensive Prediction of the Color Optical Properties of Anthocyanins in Solution. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3816-3822.	2.5	43
43	Optical properties of anthocyanins in the gas phase. <i>Chemical Physics Letters</i> , 2015, 618, 24-29.	2.7	6
44	Microscopic theory and quantum simulation of atomic heat transport. <i>Nature Physics</i> , 2015, 12, 80-84.	16.0	120
45	Approximate treatment of semicore states in GW calculations with application to Au clusters. <i>Journal of Chemical Physics</i> , 2014, 140, .	2.8	5
46	Clozapine effects on adenylyl cyclase activity and serotonin type 1A receptors in human brain post-mortem. <i>Journal of Psychopharmacology</i> , 2014, 28, 320-328.	4.8	8
47	turboTDDFT 2.0â€”Hybrid functionals and new algorithms within time-dependent density-functional perturbation theory. <i>Computer Physics Communications</i> , 2014, 185, 2080-2089.	7.6	69
48	Dimorphic changes of some features of loving relationships during long-term use of antidepressants in depressed outpatients. <i>Journal of Affective Disorders</i> , 2014, 166, 151-155.	4.5	12
49	Energy-level alignment in organic dye-sensitized TiO <sub>2</sub> from GW calculations. <i>Journal of Chemical Physics</i> , 2013, 139, .	2.8	57
50	Electron energy loss and inelastic x-ray scattering cross sections from time-dependent density-functional perturbation theory. <i>Physical Review B</i> , 2013, 88, .	3.4	44
51	Serotonin receptor of type 6 (5-HT <sub>6</sub> ) in human prefrontal cortex and hippocampus post-mortem: An immunohistochemical and immunofluorescence study. <i>Neurochemistry International</i> , 2013, 62, 182-188.	3.5	33
52	The neurobiology of moral sense: facts or hypotheses?. <i>Annals of General Psychiatry</i> , 2013, 12, 6.	2.3	30
53	The expression of platelet serotonin transporter (SERT) in human obesity. <i>BMC Neuroscience</i> , 2013, 14, .	2.1	23
54	Non-Monoaminergic Targets for the Development of Antidepressants: Focus on Neuropeptides. <i>Mini-Reviews in Medicinal Chemistry</i> , 2013, 13, 2-10.	2.9	29

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55	Serotonin Receptors of Type 6 (5-HT <sub>6</sub> ): From Neuroscience to Clinical Pharmacology. <i>Current Medicinal Chemistry</i> , 2013, 20, 371-377.	2.8	21
56	Absolute Transition Rates for Rare Events from Dynamical Decoupling of Reaction Variables. <i>Physical Review Letters</i> , 2012, 109, .	8.2	10
57	Plasma clomipramine levels in adult patients with obsessive-compulsive disorder. <i>International Clinical Psychopharmacology</i> , 2012, 27, 55-60.	1.2	7
58	A link between oxytocin and serotonin in humans: Supporting evidence from peripheral markers. <i>European Neuropsychopharmacology</i> , 2012, 22, 578-583.	1.0	35
59	Plasma fluvoxamine levels and OCD symptoms/response in adult patients. <i>Human Psychopharmacology</i> , 2012, 27, 397-402.	1.7	9
60	Distribution of Serotonin Receptor of Type 6 (5-HT <sub>6</sub> ) in Human Brain Post-mortem. A Pharmacology, Autoradiography and Immunohistochemistry Study. <i>Neurochemical Research</i> , 2012, 37, 920-927.	3.4	29
61	Itinerant ferromagnetic phase of the Hubbard model. <i>Physical Review B</i> , 2011, 83, .	3.4	31
62	Surface Precursors and Reaction Mechanisms for the Thermal Reduction of Graphene Basal Surfaces Oxidized by Atomic Oxygen. <i>Journal of Physical Chemistry C</i> , 2011, 115, 4730-4737.	3.1	106
63	Oxygen Dissociation by Concerted Action of Di-Iron Centers in Metal-Organic Coordination Networks at Surfaces: Modeling Non-Heme Iron Enzymes. <i>Nano Letters</i> , 2011, 11, 5414-5420.	8.7	75
64	Dielectric and Thermal Effects on the Optical Properties of Natural Dyes: A Case Study on Solvated Cyanin. <i>Journal of the American Chemical Society</i> , 2011, 133, 15425-15433.	15.0	55
65	turboTDDFT – A code for the simulation of molecular spectra using the Liouville-Lanczos approach to time-dependent density-functional perturbation theory. <i>Computer Physics Communications</i> , 2011, 182, 1744-1754.	7.6	197
66	Effects of cognitive-behavioral therapy on Eating Disorders: Neurotransmitter secretory response to treatment. <i>Psychoneuroendocrinology</i> , 2010, 35, 729-737.	2.7	12
67	Order-disorder phase boundary between ice VII and VIII obtained by first principles. <i>Chemical Physics Letters</i> , 2010, 499, 236-240.	2.7	46
68	Romantic Attachment and Subtypes/Dimensions of Jealousy. <i>Clinical Practice and Epidemiology in Mental Health</i> , 2010, 06, 53-58.	2.0	31
69	Harnessing molecular excited states with Lanczos chains. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 074204.	2.3	15
70	Reptation quantum Monte Carlo algorithm for lattice Hamiltonians with a directed-update scheme. <i>Physical Review E</i> , 2010, 82, .	2.1	15
71	Metallization of the C <sub>60</sub> /Rh(100) interface revealed by valence photoelectron spectroscopy and density functional theory calculations. <i>Journal of Chemical Physics</i> , 2010, 132, .	2.8	5
72	Male axillary extracts modify the affinity of the platelet serotonin transporter and impulsiveness in women. <i>Physiology and Behavior</i> , 2010, 100, 364-368.	2.2	9

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73	Alterations of the dopamine transporter in resting lymphocytes of patients with different psychotic disorders. <i>Psychiatry Research</i> , 2010, 175, 54-57.	3.1	20
74	GW quasiparticle spectra from occupied states only. <i>Physical Review B</i> , 2010, 81, .	3.4	184
75	Romantic Attachment and Subtypes/Dimensions of Jealousy. <i>Clinical Practice and Epidemiology in Mental Health</i> , 2010, 1, 53-58.	2.0	2
76	Zero-temperature dynamics of solid H <sub>4</sub> from quantum Monte Carlo simulations. <i>Physical Review B</i> , 2009, 80, .	3.4	8
77	Time-dependent density functional theory study of squaraine dye-sensitized solar cells. <i>Chemical Physics Letters</i> , 2009, 475, 49-53.	2.7	85
78	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 395502.	2.3	23,463
79	[ <sup>3</sup> H]-YM-09151-2 binding sites in human brain postmortem. <i>Neurochemistry International</i> , 2009, 55, 643-647.	3.5	10
80	Normalisation of immune cell imbalance after pharmacological treatments of patients suffering from obsessive-compulsive disorder. <i>Journal of Psychopharmacology</i> , 2009, 23, 567-573.	4.8	19
81	Optimal representation of the polarization propagator for large-scale GW calculations. <i>Physical Review B</i> , 2009, 79, .	3.4	113
82	Molecular design of photoactive acenes for organic photovoltaics. <i>Journal of Chemical Physics</i> , 2009, 130, .	2.8	21
83	What determines the catalyst's selectivity in the ethylene epoxidation reaction. <i>Journal of Catalysis</i> , 2008, 254, 304-309.	6.5	79
84	Anti-inflammatory activity of the extract, fractions and amides from the leaves of <i>Piper ovatum</i> Vahl (Piperaceae). <i>Journal of Ethnopharmacology</i> , 2008, 116, 569-573.	5.3	42
85	Adsorption of chlorine on Ag(111): No subsurface Cl at low coverage. <i>Physical Review B</i> , 2008, 78, .	3.4	39
86	Electronic Structure of Surface-supported Bis(phthalocyaninato) terbium(III) Single Molecular Magnets. <i>Nano Letters</i> , 2008, 8, 3364-3368.	8.7	191
87	Ab initio simulation of photoemission spectroscopy in solids: Plane-wave pseudopotential approach with applications to normal-emission spectra of Cu(001) and Cu(111). <i>Physical Review B</i> , 2008, 77, .	3.4	9
88	Activated Adsorption of Ethylene on Atomic-Oxygen-Covered Ag(100) and Ag(210): Formation of an Oxametallacycle. <i>Journal of Physical Chemistry C</i> , 2008, 112, 1019-1027.	3.1	26
89	Turbo charging time-dependent density-functional theory with Lanczos chains. <i>Journal of Chemical Physics</i> , 2008, 128, .	2.8	256
90	Properties of Pt-supported Co nanomagnets from relativistic density functional theory calculations. <i>Physical Review B</i> , 2008, 78, .	3.4	27

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91	Characterizing In and N impurities in GaAs from a computer simulation of (110) cross-sectional STM images. <i>Physical Review B</i> , 2007, 75, .	3.4	6
92	Thermal balneotherapy induces changes of the platelet serotonin transporter in healthy subjects. <i>Progress in Neuro-Psychopharmacology and Biological Psychiatry</i> , 2007, 31, 1436-1439.	3.8	17
93	Defect-Controlled Transport Properties of Metallic Atoms along Carbon Nanotube Surfaces. <i>Physical Review Letters</i> , 2007, 99, .	8.2	33
94	Hydrogen and Coordination Bonding Supramolecular Structures of Trimesic Acid on Cu(110). <i>Journal of Physical Chemistry A</i> , 2007, 111, 12589-12603.	2.5	121
95	Computational Spectroscopy of Carbon Monoxide Isotopomers in Helium Clusters. <i>Journal of Physical Chemistry A</i> , 2007, 111, 7640-7645.	2.5	26
96	Unraveling Excited States of Doped Helium Clusters. <i>Journal of Physical Chemistry A</i> , 2007, 111, 12749-12753.	2.5	4
97	Presence of D4 dopamine receptors in human prefrontal cortex: a postmortem study. <i>Revista Brasileira De Psiquiatria</i> , 2007, 29, 148-152.	0.9	4
98	SiC1 $\hat{\sim}$ xO2 alloys: A possible route to stabilize carbon-based silica-like solids?. <i>Solid State Communications</i> , 2007, 144, 273-276.	2.3	20
99	Tubby protein in human lymphocytes from normal weight and obese subjects. <i>Clinical Biochemistry</i> , 2007, 40, 806-809.	1.8	4
100	Presence and Characterization of the Dopamine Transporter in Human Resting Lymphocytes. <i>Neurochemical Research</i> , 2007, 33, 1011-1016.	3.4	13
101	Efficient Approach to Time-Dependent Density-Functional Perturbation Theory for Optical Spectroscopy. <i>Physical Review Letters</i> , 2006, 96, .	8.2	223
102	Interaction of Hydrogen with Cerium Oxide Surfaces: a Quantum Mechanical Computational Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 19380-19385.	2.7	92
103	DFT Study of a Weakly $\hat{\text{I}}$ -Bonded C2H4 on Oxygen-Covered Ag(100). <i>Journal of Physical Chemistry B</i> , 2006, 110, 367-376.	2.7	22
104	Monitoring Two-Dimensional Coordination Reactions: A Directed Assembly of Co $\hat{\sim}$ Terephthalate Nanosystems on Au(111). <i>Journal of Physical Chemistry B</i> , 2006, 110, 5627-5632.	2.7	74
105	Binding of 3H-WIN-35,428 and 125I-RTI-121 to Human Platelet Membranes. <i>Neurochemical Research</i> , 2006, 31, 361-365.	3.4	13
106	Common Alterations in the Serotonin Transporter in Platelets and Lymphocytes of Psychotic Patients. <i>Pharmacopsychiatry</i> , 2006, 39, 35-38.	1.8	15
107	Title is missing!. <i>Clinical Practice and Epidemiology in Mental Health</i> , 2006, 2, 28.	2.0	104
108	Methane Dehydrogenation on Rh@Cu(111): A First-Principles Study of a Model Catalyst. <i>Journal of the American Chemical Society</i> , 2006, 128, 12448-12454.	15.0	66

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109	Cross-sectional imaging of sharp Si interlayers embedded in gallium arsenide. Applied Physics Letters, 2006, 88, 022115.	3.0	4
110	On-surface and sub-surface oxygen adsorption on Ag(210): Vibrational properties. Surface Science, 2005, 587, 50-54.	1.7	12
111	Computational spectroscopy of doped He clusters. Computer Physics Communications, 2005, 169, 404-407.	7.6	21
112	Characterization of Si-doped GaAs cross-sectional surfaces via ab initio simulations. Physical Review B, 2005, 72, .	3.4	14
113	Computer Simulation of Quantum Melting in Hydrogen Clusters. ChemPhysChem, 2005, 6, 1884-1888.	1.9	30
114	Templated Growth of Metal-Organic Coordination Chains at Surfaces. Angewandte Chemie - International Edition, 2005, 44, 6142-6145.	14.4	131
115	Templated Growth of Metal-Organic Coordination Chains at Surfaces. Angewandte Chemie, 2005, 117, 6298-6301.	1.4	29
116	Energetically Driven Reorganization of a Modified Catalytic Surface under Reaction Conditions. Journal of the American Chemical Society, 2005, 127, 2351-2357.	15.0	38
117	Computational spectroscopy of helium-solvated molecules: Effective inertia, from small He clusters toward the nanodroplet regime. Journal of Chemical Physics, 2005, 123, 114306.	2.8	57
118	Spin-Flop Ordering from Frustrated Ferro- and Antiferromagnetic Interactions: A Combined Theoretical and Experimental Study of a Mn/Fe(100) Monolayer. Physical Review Letters, 2005, 95, .	8.2	28
119	Taming multiple valency with density functionals: A case study of defective ceria. Physical Review B, 2005, 71, .	3.4	405
120	First-principles codes for computational crystallography in the Quantum-ESPRESSO package. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	2.5	232
121	Decreased density of peripheral benzodiazepine receptors in psychiatric patients after a suicide attempt. Life Sciences, 2005, 77, 3268-3275.	4.5	9
122	Electronic and Atomistic Structures of Clean and Reduced Ceria Surfaces. Journal of Physical Chemistry B, 2005, 109, 22860-22867.	2.7	388
123	Reply to 'Comment on "Taming multiple valency with density functionals: A case study of defective ceria"' Physical Review B, 2005, 72, .	3.4	191
124	Changes in peripheral benzodiazepine receptors in patients with bipolar disorder. Neuropsychiatric Disease and Treatment, 2005, 1, 151-154.	4.2	4
125	Anomalous Pressure-Induced Transition(s) in Ice XI. Physical Review Letters, 2004, 92, .	8.2	38
126	Adsorption of ethylene on stepped Ag() surfaces. Surface Science, 2004, 566-568, 1018-1023.	1.7	16

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127	Engineering the Reactivity of Metal Catalysts: A Model Study of Methane Dehydrogenation on Rh(111). Journal of the American Chemical Society, 2004, 126, 16732-16733.	15.0	84
128	Rotational dynamics of CO solvated in small He clusters: A quantum Monte Carlo study. Journal of Chemical Physics, 2004, 120, 9071-9076.	2.8	46
129	Oxygen vibrations in O <sub>2</sub> /Ag(001). Surface Science, 2003, 530, 26-36.	1.7	18
130	Co-adsorption of ethylene and oxygen on the Ag(001) surface. Surface Science, 2003, 532-535, 191-197.	1.7	14
131	Structure, Rotational Dynamics, and Superfluidity of Small OCS-Doped He Clusters. Physical Review Letters, 2003, 90, .	8.2	112
132	Platelet Serotonin Transporter in Patients With Diarrhea-Predominant Irritable Bowel Syndrome Both Before and After Treatment With Alosetron. American Journal of Gastroenterology, 2003, 98, 2705-2711.	0.7	55
133	Platelet serotonin transporter in patients with diarrhea-predominant irritable bowel syndrome both before and after treatment with alosetron. American Journal of Gastroenterology, 2003, 98, 2705-2711.	0.7	0
134	The Interaction of Ethylene with Perfect and Defective Ag(001) Surfaces. Journal of Physical Chemistry B, 2002, 106, 9839-9846.	2.7	45
135	Adsorption of atomic oxygen on Ag(): a study based on density-functional theory. Surface Science, 2002, 501, 182-190.	1.7	51
136	Decreased inhibitory activity of PKC in OCD patients after six months of treatment. Psychoneuroendocrinology, 2002, 27, 769-776.	2.7	12
137	Phonons and related crystal properties from density-functional perturbation theory. Reviews of Modern Physics, 2001, 73, 515-562.	40.8	9,398
138	First principles thermoelasticity of MgSiO <sub>3</sub> -perovskite: Consequences for the inferred properties of the lower mantle. Geophysical Research Letters, 2001, 28, 2699-2702.	4.1	57
139	Decreased platelet [3H]paroxetine binding sites in suicide attempters. Psychiatry Research, 2001, 103, 125-131.	3.1	20
140	Oxygen Self-Diffusion in $\alpha$ -Quartz. Physical Review Letters, 2001, 86, 4564-4567.	8.2	60
141	Title is missing!. Neurochemical Research, 2001, 26, 187-190.	3.4	23
142	Increased Density of the Platelet Serotonin Transporter in Autism. Pharmacopsychiatry, 2000, 33, 165-168.	1.8	45
143	Effects of isotopic disorder on the Raman spectra of crystals: Theory and ab initio calculations for diamond and germanium. Physical Review B, 2000, 61, 9387-9392.	3.4	21
144	Magnons in real materials from density-functional theory. Physical Review B, 2000, 61, R6459-R6462.	3.4	126

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145	Effects of isotopic disorder on the Raman spectra of crystals: theory and ab initio calculations for diamond and germanium. <i>Computational Materials Science</i> , 2000, 17, 395-399.	3.2	8
146	Thermodynamic properties and lattice dynamics of silver at high pressure: A first-principles study. <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , 1999, 79, 911-919.	0.6	20
147	Reptation Quantum Monte Carlo: A Method for Unbiased Ground-State Averages and Imaginary-Time Correlations. <i>Physical Review Letters</i> , 1999, 82, 4745-4748.	8.2	209
148	Effects of disorder on the optical gap of (Zn,Mg)(S,Se). <i>Applied Physics Letters</i> , 1999, 75, 2746-2748.	3.0	14
149	High-pressure thermal expansion, bulk modulus, and phonon structure of diamond. <i>Physical Review B</i> , 1999, 60, 9444-9449.	3.4	92
150	Temperature-dependent surface relaxations of Ag(111). <i>Physical Review B</i> , 1999, 59, 970-974.	3.4	58
151	Platelet [3H]paroxetine binding in patients with OCD-related disorders. <i>Psychiatry Research</i> , 1999, 89, 223-228.	3.1	42
152	The reconstruction of nickel and rhodium (001) surfaces upon carbon, nitrogen or oxygen adsorptions. <i>Surface Science</i> , 1999, 437, 18-28.	1.7	37
153	First-principles calculation of the thermal properties of silver. <i>Physical Review B</i> , 1999, 59, 965-969.	3.4	132
154	High Pressure Lattice Instabilities and Structural Phase Transformations in Solids from Ab-Initio Lattice Dynamics. <i>Materials Research Society Symposia Proceedings</i> , 1998, 499, .	0.1	2
155	Presence and Characterization of the Serotonin Transporter in Human Resting Lymphocytes. <i>Neuropsychopharmacology</i> , 1998, 19, 154-159.	5.4	31
156	$\hat{\mu}_T^2$ phase transition in tin: A theoretical study based on density-functional perturbation theory. <i>Physical Review B</i> , 1998, 57, 10421-10423.	3.4	107
157	Dynamical-charge neutrality at a crystal surface. <i>Physical Review B</i> , 1998, 57, 5742-5745.	3.4	19
158	Vibrational broadening of x-ray emission spectra: A first-principles study on diamond. <i>Physical Review B</i> , 1997, 55, 9649-9658.	3.4	22
159	The surface chemistry of metal-oxygen interactions: a first-principles study of O:Rh(110). <i>Surface Science</i> , 1997, 370, 166-178.	1.7	35
160	The structure and phase stability of CO adsorbates on Rh(110). <i>Surface Science</i> , 1997, 382, L666-L671.	1.7	9
161	Theory of the Anomalous Rayleigh Dispersion at H/W(110) Surfaces. <i>Physical Review Letters</i> , 1996, 77, 2491-2494.	8.2	53
162	The phonon spectra of LiH and LiD from density-functional perturbation theory. <i>Solid State Communications</i> , 1996, 98, 203-207.	2.3	35

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163	InAs/GaSb(001) valence band offset: Independence of interface composition and strain. Applied Physics Letters, 1996, 69, 3218-3220.	3.0	13
164	Formation Energy, Stress, and Relaxations of Low-Index Rhodium Surfaces. Materials Research Society Symposia Proceedings, 1995, 408, .	0.1	4
165	High-pressure low-symmetry phases of cesium halides. Physical Review B, 1995, 51, 8060-8068.	3.4	23
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