Stefano Baroni

List of Publications by Year in Descending Order

152 papers	29,986 citations	50 h-index	154 g-index
154 ext. papers	34,440 ext. citations	5.2 avg, IF	6.56 L-index

#	Paper	IF	Citations
152	Temperature- and vacancy-concentration-dependence of heat transport in Li3ClO from multi-method numerical simulations. *Npj Computational Materials*, **2022**, 8,	10.9	1
151	Heat transport in liquid water from first-principles and deep neural network simulations. *Physical Review B*, **2021**, 104,	3.3	4
150	Thermal and Tidal Evolution of Uranus with a Growing Frozen Core. *Planetary Science Journal*, **2021**, 2, 222	2.9	5
149	Discovery of a natural cyan blue: A unique food-sourced anthocyanin could replace synthetic brilliant blue. *Science Advances*, **2021**, 7,	14.3	8
148	Invariance principles in the theory and computation of transport coefficients. *European Physical Journal B*, **2021**, 94, 160	1.2	3
147	QEHeat: An open-source energy flux calculator for the computation of heat-transport coefficients from first principles. *Computer Physics Communications*, **2021**, 269, 108090	4.2	3
146	Gauge Fixing for Heat-Transport Simulations. *Journal of Chemical Theory and Computation*, **2020**, 16, 3352-3362	6.4	6
145	Heat Transport in Insulators from Ab Initio Green-Kubo Theory **2020**, 809-844		1
144	Heat and charge transport in HO at ice-giant conditions from ab initio molecular dynamics simulations. *Nature Communications*, **2020**, 11, 3605	17.4	8
143	Oxidation States, Thouless Pumps, and Nontrivial Ionic Transport in Nonstoichiometric Electrolytes. *Physical Review X*, **2020**, 10,	9.1	3
142	Electron energy loss spectroscopy of bulk gold with ultrasoft pseudopotentials and the Liouville-Lanczos method. *Physical Review B*, **2020**, 102,	3.3	1
141	Quantum ESPRESSO toward the exascale. *Journal of Chemical Physics*, **2020**, 152, 154105	3.9	227
140	Modeling heat transport in crystals and glasses from a unified lattice-dynamical approach. *Nature Communications*, **2019**, 10, 3853	17.4	39
139	Fast hybrid density-functional computations using plane-wave basis sets. *Electronic Structure*, **2019**, 1, 015009	2.6	16
138	Unraveling the molecular mechanisms of color expression in anthocyanins. *Physical Chemistry Chemical Physics*, **2019**, 21, 8757-8766	3.6	10
137	Theory and Numerical Simulation of Heat Transport in Multicomponent Systems. *Physical Review Letters*, **2019**, 122, 255901	7.4	13
136	Topological quantization and gauge invariance of charge transport in liquid insulators. *Nature Physics*, **2019**, 15, 967-972	16.2	14

135	Spin dynamics from time-dependent density functional perturbation theory. *European Physical Journal B*, **2018**, 91, 1	1.2	7
134	Heat Transport in Insulators from Ab Initio Green-Kubo Theory **2018**, 1-36		9
133	Ab initio study of electron energy loss spectra of bulk bismuth up to 100 eV. *Physical Review B*, **2017**, 95,	3.3	4
132	Accurate thermal conductivities from optimally short molecular dynamics simulations. *Scientific Reports*, **2017**, 7, 15835	4.9	28
131	Microscopic theory and quantum simulation of atomic heat transport. *Nature Physics*, **2016**, 12, 80-84	16.2	63
130	Sampling Molecular Conformers in Solution with Quantum Mechanical Accuracy at a Nearly Molecular-Mechanics Cost. *Journal of Chemical Theory and Computation*, **2016**, 12, 4385-9	6.4	14
129	Multimodel Approach to the Optical Properties of Molecular Dyes in Solution. *Journal of Chemical Theory and Computation*, **2016**, 12, 4423-9	6.4	10
128	Gauge Invariance of Thermal Transport Coefficients. *Journal of Low Temperature Physics*, **2016**, 185, 79-86	1.3	19
127	Self-consistent continuum solvation for optical absorption of complex molecular systems in solution. *Journal of Chemical Physics*, **2015**, 142, 034111	3.9	14
126	Accurate and inexpensive prediction of the color optical properties of anthocyanins in solution. *Journal of Physical Chemistry A*, **2015**, 119, 3816-22	2.8	28
125	Optical properties of anthocyanins in the gas phase. *Chemical Physics Letters*, **2015**, 618, 24-29	2.5	3
124	turboEELS—A code for the simulation of the electron energy loss and inelastic X-ray scattering spectra using the Liouville–Lanczos approach to time-dependent density-functional perturbation theory. *Computer Physics Communications*, **2015**, 196, 460-469	4.2	23
123	Approximate treatment of semicore states in GW calculations with application to Au clusters. *Journal of Chemical Physics*, **2014**, 140, 124101	3.9	5
122	turboTDDFT 2.0—Hybrid functionals and new algorithms within time-dependent density-functional perturbation theory. *Computer Physics Communications*, **2014**, 185, 2080-2089	4.2	43
121	Energy-level alignment in organic dye-sensitized TiO2 from GW calculations. *Journal of Chemical Physics*, **2013**, 139, 014709	3.9	43
120	Electron energy loss and inelastic x-ray scattering cross sections from time-dependent density-functional perturbation theory. *Physical Review B*, **2013**, 88,	3.3	19
119	Absolute transition rates for rare events from dynamical decoupling of reaction variables. *Physical Review Letters*, **2012**, 109, 150601	7.4	8
118	The Liouville-Lanczos Approach to Time-Dependent Density-Functional (Perturbation) Theory. *Lecture Notes in Physics*, **2012**, 375-390	0.8	6

117	Itinerant ferromagnetic phase of the Hubbard model. *Physical Review B*, **2011**, 83,	3.3	21
116	Surface Precursors and Reaction Mechanisms for the Thermal Reduction of Graphene Basal Surfaces Oxidized by Atomic Oxygen. *Journal of Physical Chemistry C*, **2011**, 115, 4730-4737	3.8	82
115	Oxygen dissociation by concerted action of di-iron centers in metal-organic coordination networks at surfaces: modeling non-heme iron enzymes. *Nano Letters*, **2011**, 11, 5414-20	11.5	60
114	Dielectric and thermal effects on the optical properties of natural dyes: a case study on solvated cyanin. *Journal of the American Chemical Society*, **2011**, 133, 15425-33	16.4	46
113	turboTDDFT A code for the simulation of molecular spectra using the Liouville anczos approach to time-dependent density-functional perturbation theory. *Computer Physics Communications*, **2011** , 182, 1744-1754	4.2	133
112	Accelerating GW Calculations with Optimal Polarizability Basis **2011**, 61-78		
111	3. Density-Functional Perturbation Theory for Quasi-Harmonic Calculations **2010**, 39-58		7
110	Harnessing molecular excited states with Lanczos chains. *Journal of Physics Condensed Matter*, **2010** , 22, 074204	1.8	14
109	Reptation quantum Monte Carlo algorithm for lattice Hamiltonians with a directed-update scheme. *Physical Review E*, **2010**, 82, 046710	2.4	11
108	Metallization of the C60/Rh(100) interface revealed by valence photoelectron spectroscopy and density functional theory calculations. *Journal of Chemical Physics*, **2010**, 132, 234710	3.9	4
107	GW quasiparticle spectra from occupied states only. *Physical Review B*, **2010**, 81,	3.3	155
106	Order isorder phase boundary between ice VII and VIII obtained by first principles. *Chemical Physics Letters*, **2010**, 499, 236-240	2.5	30
105	Zero-temperature dynamics of solid H4e from quantum Monte Carlo simulations. *Physical Review B*, **2009**, 80,	3.3	8
104	Time-dependent density functional theory study of squaraine dye-sensitized solar cells. *Chemical Physics Letters*, **2009**, 475, 49-53	2.5	79
103	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. *Journal of Physics Condensed Matter*, **2009**, 21, 395502	1.8	13251
102	Optimal representation of the polarization propagator for large-scale GW calculations. *Physical Review B*, **2009**, 79,	3.3	95
101	Molecular design of photoactive acenes for organic photovoltaics. *Journal of Chemical Physics*, **2009** , 130, 194701	3.9	18
100	Ab initio studies of structural and electronic properties **2008**, 17-54		2

99	Adsorption of chlorine on Ag(111): No subsurface Cl at low coverage. *Physical Review B*, **2008**, 78,	3.3	33
98	Electronic structure of surface-supported bis(phthalocyaninato) terbium(III) single molecular magnets. *Nano Letters*, **2008**, 8, 3364-8	11.5	165
97	Ab initio simulation of photoemission spectroscopy in solids: Plane-wave pseudopotential approach with applications to normal-emission spectra of Cu(001) and Cu(111). *Physical Review B*, **2008**, 77,	3.3	9
96	Activated Adsorption of Ethylene on Atomic-Oxygen-Covered Ag(100) and Ag(210): Formation of an Oxametallacycle. *Journal of Physical Chemistry C*, **2008**, 112, 1019-1027	3.8	17
95	Turbo charging time-dependent density-functional theory with Lanczos chains. *Journal of Chemical Physics*, **2008**, 128, 154105	3.9	207
94	Hydrogen and coordination bonding supramolecular structures of trimesic acid on Cu(110). *Journal of Physical Chemistry A*, **2007**, 111, 12589-603	2.8	107
93	Computational spectroscopy of carbon monoxide isotopomers in helium clusters. *Journal of Physical Chemistry A*, **2007**, 111, 7640-5	2.8	26
92	Unraveling excited states of doped helium clusters. *Journal of Physical Chemistry A*, **2007**, 111, 12749-53	2.8	4
91	SixC1⊠O2 alloys: A possible route to stabilize carbon-based silica-like solids?. *Solid State Communications*, **2007**, 144, 273-276	1.6	14
90	Characterizing In and N impurities in GaAs from ab initio computer simulation of (110) cross-sectional STM images. *Physical Review B*, **2007**, 75,	3.3	5
89	Methane dehydrogenation on Rh@Cu(111): a first-principles study of a model catalyst. *Journal of the American Chemical Society*, **2006**, 128, 12448-54	16.4	48
88	Cross-sectional imaging of sharp Si interlayers embedded in gallium arsenide. *Applied Physics Letters*, **2006**, 88, 022115	3.4	3
87	Efficient approach to time-dependent density-functional perturbation theory for optical spectroscopy. *Physical Review Letters*, **2006**, 96, 113001	7.4	166
86	Interaction of hydrogen with cerium oxide surfaces: a quantum mechanical computational study. *Journal of Physical Chemistry B*, **2006**, 110, 19380-5	3.4	77
85	DFT study of a weakly pi-bonded C2H4 on oxygen-covered Ag(100). *Journal of Physical Chemistry B*, **2006**, 110, 367-76	3.4	18
84	Monitoring two-dimensional coordination reactions: directed assembly of co-terephthalate nanosystems on Au(111). *Journal of Physical Chemistry B*, **2006**, 110, 5627-32	3.4	72
83	Taming multiple valency with density functionals: A case study of defective ceria. *Physical Review B*, **2005**, 71,	3.3	347
82	First-principles codes for computational crystallography in the Quantum-ESPRESSO package. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2005**, 220,	1	122

81	Electronic and atomistic structures of clean and reduced ceria surfaces. *Journal of Physical Chemistry B*, **2005**, 109, 22860-7	3.4	314
80	Reply to Comment on Taming multiple valency with density functionals: A case study of defective ceria' *Physical Review B*, **2005**, 72,	3.3	161
79	On-surface and sub-surface oxygen adsorption on Ag(210): Vibrational properties. *Surface Science*, **2005**, 587, 50-54	1.8	10
78	Computational spectroscopy of doped He clusters. *Computer Physics Communications*, **2005**, 169, 404-407	4.2	18
77	Characterization of Si-doped GaAs cross-sectional surfaces via ab initio simulations. *Physical Review B*, **2005**, 72,	3.3	13
76	Computer simulation of quantum melting in hydrogen clusters. *ChemPhysChem*, **2005**, 6, 1884-8	3.2	30
75	Templated growth of metal-organic coordination chains at surfaces. *Angewandte Chemie - International Edition*, **2005**, 44, 6142-5	16.4	118
74	Energetically driven reorganization of a modified catalytic surface under reaction conditions. *Journal of the American Chemical Society*, **2005**, 127, 2351-7	16.4	27
73	Computational spectroscopy of helium-solvated molecules: effective inertia, from small He clusters toward the nanodroplet regime. *Journal of Chemical Physics*, **2005**, 123, 114306	3.9	57
72	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, 117201	7.4	26
71	Density-Functional Perturbation Theory **2005**, 195-214		9
70	Anomalous pressure-induced transition(s) in ice XI. *Physical Review Letters*, **2004**, 92, 105502	7.4	35
69	Adsorption of ethylene on stepped Ag() surfaces. *Surface Science*, **2004**, 566-568, 1018-1023	1.8	15
68	Engineering the reactivity of metal catalysts: a model study of methane dehydrogenation on Rh(111). *Journal of the American Chemical Society*, **2004**, 126, 16732-3	16.4	63
67	Rotational dynamics of CO solvated in small He clusters: a quantum Monte Carlo study. *Journal of Chemical Physics*, **2004**, 120, 9071-6	3.9	45
66	Oxygen vibrations in O/Ag(0 0 1). *Surface Science*, **2003**, 530, 26-36	1.8	13
65	Co-adsorption of ethylene and oxygen on the Ag(001) surface. *Surface Science*, **2003**, 532-535, 191-197	1.8	14
64	Structure, rotational dynamics, and superfluidity of small OCS-doped He clusters. *Physical Review Letters*, **2003**, 90, 143401	7.4	104

63	The Interaction of Ethylene with Perfect and Defective Ag(001) Surfaces. *Journal of Physical Chemistry B*, **2002**, 106, 9839-9846	3.4	43
62	Adsorption of atomic oxygen on Ag(): a study based on density-functional theory. *Surface Science*, **2002**, 501, 182-190	1.8	42
61	Phonons and related crystal properties from density-functional perturbation theory. *Reviews of Modern Physics*, **2001**, 73, 515-562	40.5	5812
60	First principles thermoelasticity of MgSiO3-perovskite: Consequences for the inferred properties of the lower mantle. *Geophysical Research Letters*, **2001**, 28, 2699-2702	4.9	49
59	Oxygen self-diffusion in alpha-quartz. *Physical Review Letters*, **2001**, 86, 4564-7	7.4	56
58	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	3.3	18
57	Magnons in real materials from density-functional theory. *Physical Review B*, **2000**, 61, R6459-R6462	3.3	85
56	Effects of isotopic disorder on the Raman spectra of crystals: theory and ab initio calculations for diamond and germanium. *Computational Materials Science*, **2000**, 17, 395-399	3.2	7
55	Thermodynamic properties and lattice dynamics of silver at high pressure: A first-principles study. *The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties*, **1999**, 79, 911-919		15
54	Reptation Quantum Monte Carlo: A Method for Unbiased Ground-State Averages and Imaginary-Time Correlations. *Physical Review Letters*, **1999**, 82, 4745-4748	7.4	184
53	Effects of disorder on the optical gap of (Zn,Mg)(S,Se). *Applied Physics Letters*, **1999**, 75, 2746-2748	3.4	13
52	High-pressure thermal expansion, bulk modulus, and phonon structure of diamond. *Physical Review B*, **1999**, 60, 9444-9449	3.3	70
51	Temperature-dependent surface relaxations of Ag(111). *Physical Review B*, **1999**, 59, 970-974	3.3	53
50	The reconstruction of nickel and rhodium (001) surfaces upon carbon, nitrogen or oxygen adsorptions. *Surface Science*, **1999**, 437, 18-28	1.8	36
49	First-principles calculation of the thermal properties of silver. *Physical Review B*, **1999**, 59, 965-969	3.3	109
48	Reptation Quantum Monte Carlo **1999**, 313-341		8
47	□-□ phase transition in tin: A theoretical study based on density-functional perturbation theory. *Physical Review B*, **1998**, 57, 10421-10423	3.3	86
46	Dynamical-charge neutrality at a crystal surface. *Physical Review B*, **1998**, 57, 5742-5745	3.3	16

45	Vibrational broadening of x-ray emission spectra: A first-principles study on diamond. *Physical Review B*, **1997**, 55, 9649-9658	3.3	19
44	High Pressure Lattice Instabilities and Structural Phase Transformations in Solids from Ab-Initio Lattice Dynamics. *Materials Research Society Symposia Proceedings*, **1997**, 499, 233		1
43	The surface chemistry of metal-oxygen interactions: a first-principles study of O:Rh(110). *Surface Science*, **1997**, 370, 166-178	1.8	33
42	The structure and phase stability of CO adsorbates on Rh(110). *Surface Science*, **1997**, 382, L666-L671	1.8	8
41	Theory of the Anomalous Rayleigh Dispersion at H/W(110) Surfaces. *Physical Review Letters*, **1996**, 77, 2491-2494	7.4	50
40	The phonon spectra of LiH and LiD from density-functional perturbation theory. *Solid State Communications*, **1996**, 98, 203-207	1.6	30
39	InAs/GaSb(001) valence-band offset: Independence of interface composition and strain. *Applied Physics Letters*, **1996**, 69, 3218-3220	3.4	12
38	High-pressure low-symmetry phases of cesium halides. *Physical Review B*, **1995**, 51, 8060-8068	3.3	22
37	Anharmonic Phonon Lifetimes in Semiconductors from Density-Functional Perturbation Theory. *Physical Review Letters*, **1995**, 75, 1819-1822	7.4	270
36	Density-functional theory of the dielectric constant: Gradient-corrected calculation for silicon. *Physical Review B*, **1994**, 49, 5323-5328	3.3	81
35	Bulk and interfacial strain in Si/Ge heterostructures. *Physical Review B*, **1994**, 49, 7490-7498	3.3	22
34	Structure and phase stability of GaxIn1-xP solid solutions from computational alchemy. *Physical Review Letters*, **1994**, 72, 4001-4004	7.4	56
33	Vibrational and dielectric properties of C60 from density-functional perturbation theory. *Journal of Chemical Physics*, **1994**, 100, 8537-8539	3.9	150
32	Dependence of the crystal lattice constant on isotopic composition: Theory and ab initio calculations for C, Si, and Ge. *Solid State Communications*, **1994**, 90, 295-297	1.6	81
31	Third-order density-functional perturbation theory: A practical implementation with applications to anharmonic couplings in Si. *Solid State Communications*, **1994**, 91, 813-816	1.6	41
30	Nonlinear piezoelectricity in CdTe. *Physical Review B*, **1993**, 47, 16252-16256	3.3	41
29	Ab initio calculation of the band offset at strained GaAs/InAs (001) heterojunctions. *Physical Review B*, **1993**, 48, 17607-17610	3.3	35
28	Auxiliary-field quantum Monte Carlo calculations for systems with long-range repulsive interactions. *Physical Review Letters*, **1993**, 71, 1148-1151	7.4	28

27	Ab initio calculation of phonon dispersions in II-VI semiconductors. *Physical Review B*, **1993**, 47, 3588-3592	3.3	196
26	Phonon softening and high-pressure low-symmetry phases of cesium iodide. *Physical Review Letters*, **1992**, 69, 1069-1072	7.4	27
25	Effects of disorder on the Raman spectra of GaAs/AlAs superlattices. *Physical Review B*, **1992**, 45, 4280-4288	3.3	87
24	Effects of disorder on the vibrational properties of SiGe alloys: Failure of mean-field approximations. *Physical Review Letters*, **1992**, 69, 1959-1962	7.4	38
23	Atomic intermixing in short period GaAs/AlAs superlattices. *Surface Science*, **1992**, 267, 171-175	1.8	24
22	Vibrational properties of isolated AlAs monolayers embedded in GaAs: a theoretical study of the effects of disorder. *Applied Surface Science*, **1992**, 56-58, 617-621	6.7	
21	Structure and Thermodynamics of SiGe Alloys from Computational Alchemy **1992**, 133-149		0
20	Tuning band offsets at semiconductor interfaces by intralayer deposition. *Physical Review B*, **1991**, 43, 7347-7350	3.3	98
19	Structure and thermodynamics of SixGe1-x alloys from ab initio Monte Carlo simulations. *Physical Review Letters*, **1991**, 66, 2116-2119	7.4	144
18	Ab initio calculation of phonon dispersions in semiconductors. *Physical Review B*, **1991**, 43, 7231-7242	3.3	1348
17	Phonon spectra of ultrathin GaAs/AlAs superlattices: An ab initio calculation. *Physical Review B*, **1990**, 41, 3870-3873	3.3	110
16	Phonon dispersions in GaxAl1-xAs alloys. *Physical Review Letters*, **1990**, 65, 84-87	7.4	104
15	Electronic structure of InP/Ga0.47In0.53As interfaces. *Physical Review B*, **1990**, 41, 12106-12110	3.3	38
14	Theory of band offsets at semiconductor heterojunctions: An ab-initio linear response approach. *Superlattices and Microstructures*, **1989**, 6, 31-37	2.8	21
13	Theoretical study of cubic versus tetragonal structures of defect zinc-blende semiconductors: CdIn2Se4. *Physical Review B*, **1989**, 40, 1725-1731	3.3	23
12	Piezoelectric properties of III-V semiconductors from first-principles linear-response theory. *Physical Review Letters*, **1989**, 62, 2853-2856	7.4	161
11	Band Offsets at Semiconductor Heterojunctions: Bulk or Interface Properties?. *NATO ASI Series Series B: Physics*, **1989**, 51-60		
10	Can We Tune the Band Offset at Semiconductor Heterojunctions?. *NATO ASI Series Series B: Physics*, **1989**, 251-271		19

9	Band offsets in lattice-matched heterojunctions: A model and first-principles calculations for GaAs/AlAs. *Physical Review Letters*, **1988**, 61, 734-737	7.4	465
8	Structural and electronic properties of spinel semiconductors: An ab initio pseudopotential study of MgIn2S. *Physical Review B*, **1988**, 38, 8258-8263	3.3	26
7	Pressure-induced structural instability of cesium halides from ab initio pseudopotential techniques. *Physical Review B*, **1987**, 35, 765-769	3.3	12
6	Elastic constants of crystals from linear-response theory. *Physical Review Letters*, **1987**, 59, 2662-2665	7.4	73
5	Green's-function approach to linear response in solids. *Physical Review Letters*, **1987**, 58, 1861-1864	7.4	1546
4	Ab initio calculation of the macroscopic dielectric constant in silicon. *Physical Review B*, **1986**, 33, 7017-7021	3.3	406
3	Exact-exchange extension of the local-spin-density approximation in atoms. II. The iron series. *Journal of Chemical Physics*, **1984**, 80, 5703-5708	3.9	26
2	Hartree-Fock energy bands in molecular crystals: Solid hydrogen in the cubic phase. *Physical Review B*, **1984**, 30, 7187-7193	3.3	7
1	Exact-exchange extension of the local-spin-density approximation in atoms: Calculation of total energies and electron affinities. *Journal of Chemical Physics*, **1983**, 79, 6140-6144	3.9	60