Stefano de Gironcoli

List of Publications by Citations

149 papers	33,206 citations	49 h-index	155 g-index
155 ext. papers	39,013 ext. citations	4.9 avg, IF	6.77 L-index

#	Paper	IF	Citations
149	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
148	Phonons and related crystal properties from density-functional perturbation theory. *Reviews of Modern Physics*, **2001**, 73, 515-562	40.5	5812
147	Advanced capabilities for materials modelling with Quantum ESPRESSO. *Journal of Physics Condensed Matter*, **2017**, 29, 465901	1.8	2275
146	Linear response approach to the calculation of the effective interaction parameters in the LDA+U method. *Physical Review B*, **2005**, 71,	3.3	2134
145	Ab initio calculation of phonon dispersions in semiconductors. *Physical Review B*, **1991**, 43, 7231-7242	3.3	1348
144	Reproducibility in density functional theory calculations of solids. *Science*, **2016**, 351, aad3000	33.3	784
143	Nonlocal van der Waals density functional made simple and efficient. *Physical Review B*, **2013**, 87,	3.3	373
142	Hubbard-corrected DFT energy functionals: The LDA+U description of correlated systems. *International Journal of Quantum Chemistry*, **2014**, 114, 14-49	2.1	359
141	Taming multiple valency with density functionals: A case study of defective ceria. *Physical Review B*, **2005**, 71,	3.3	347
140	Electronic and atomistic structures of clean and reduced ceria surfaces. *Journal of Physical Chemistry B*, **2005**, 109, 22860-7	3.4	314
139	Lattice dynamics of metals from density-functional perturbation theory. *Physical Review B*, **1995**, 51, 6773-6776	3.3	232
138	High-pressure lattice dynamics and thermoelasticity of MgO. *Physical Review B*, **2000**, 61, 8793-8800	3.3	229
137	Quantum ESPRESSO toward the exascale. *Journal of Chemical Physics*, **2020**, 152, 154105	3.9	227
136	First-principles determination of elastic anisotropy and wave velocities of MgO at lower mantle conditions. *Science*, **1999**, 286, 1705-7	33.3	218
135	Spin transition in magnesiowüstite in earth's lower mantle. *Physical Review Letters*, **2006**, 96, 198501	7.4	208
134	Ab initio calculation of phonon dispersions in II-VI semiconductors. *Physical Review B*, **1993**, 47, 3588-3592	3.3	196
133	Thermoelastic properties of MgSiO(3)-perovskite: insights on the nature of the Earth's lower mantle. *Physical Review Letters*, **2004**, 92, 018501	7.4	179

132	Reply to Comment on Taming multiple valency with density functionals: A case study of defective ceria' *Physical Review B*, **2005**, 72,	3.3	161
131	Piezoelectric properties of III-V semiconductors from first-principles linear-response theory. *Physical Review Letters*, **1989**, 62, 2853-2856	7.4	161
130	Structure and thermodynamics of SixGe1-x alloys from ab initio Monte Carlo simulations. *Physical Review Letters*, **1991**, 66, 2116-2119	7.4	144
129	First-principles codes for computational crystallography in the Quantum-ESPRESSO package. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2005**, 220,	1	122
128	Templated growth of metal-organic coordination chains at surfaces. *Angewandte Chemie - International Edition*, **2005**, 44, 6142-5	16.4	118
127	Ab initio lattice dynamics of MgSiO3 perovskite at high pressure. *Physical Review B*, **2000**, 62, 14750-14756	3.3	116
126	Efficient calculation of exact exchange and RPA correlation energies in the adiabatic-connection fluctuation-dissipation theory. *Physical Review B*, **2009**, 79,	3.3	109
125	First-principles calculation of the thermal properties of silver. *Physical Review B*, **1999**, 59, 965-969	3.3	109
124	Hydrogen and coordination bonding supramolecular structures of trimesic acid on Cu(110). *Journal of Physical Chemistry A*, **2007**, 111, 12589-603	2.8	107
123	Phonon dispersions in GaxAl1-xAs alloys. *Physical Review Letters*, **1990**, 65, 84-87	7.4	104
122	Ab initio calculation of the thermal properties of Cu: Performance of the LDA and GGA. *Physical Review B*, **2002**, 65,	3.3	91
121	Effects of disorder on the Raman spectra of GaAs/AlAs superlattices. *Physical Review B*, **1992**, 45, 4280-4288	3.3	87
120	->phase transition in tin: A theoretical study based on density-functional perturbation theory. *Physical Review B*, **1998**, 57, 10421-10423	3.3	86
119	Interaction of hydrogen with cerium oxide surfaces: a quantum mechanical computational study. *Journal of Physical Chemistry B*, **2006**, 110, 19380-5	3.4	77
118	Ab initio phonon dispersions of Fe and Ni. *Physical Review B*, **2000**, 62, 273-277	3.3	77
117	Phonons in Si-Ge systems: An ab initio interatomic-force-constant approach. *Physical Review B*, **1992**, 46, 2412-2419	3.3	77
116	High-pressure thermal expansion, bulk modulus, and phonon structure of diamond. *Physical Review B*, **1999**, 60, 9444-9449	3.3	70
115	In-plane Raman scattering of (001)-Si/Ge superlattices: Theory and experiment. *Physical Review B*, **1994**, 49, 5406-5414	3.3	70

114	Vacancy self-diffusion parameters in tungsten: Finite electron-temperature LDA calculations. *Physical Review B*, **1998**, 57, 11184-11192	3.3	69
113	Successful a priori modeling of CO adsorption on Pt(111) using periodic hybrid density functional theory. *Journal of the American Chemical Society*, **2007**, 129, 10402-7	16.4	67
112	Structural, electronic, and magnetic properties of Fe2SiO4 fayalite: Comparison of LDA and GGA results. *Physical Review B*, **2003**, 67,	3.3	65
111	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
110	Vibrational properties of MnO and NiO from DFT +U-based density functional perturbation theory. *Physical Review B*, **2011**, 84,	3.3	62
109	Phonon Softening and Superconductivity in Tellurium under Pressure. *Physical Review Letters*, **1996** , 77, 1151-1154	7.4	59
108	Isobaric first-principles molecular dynamics of liquid water with nonlocal van der Waals interactions. *Journal of Chemical Physics*, **2015**, 142, 034501	3.9	57
107	What determines the catalyst's selectivity in the ethylene epoxidation reaction. *Journal of Catalysis*, **2008**, 254, 304-309	7.3	57
106	Structure and phase stability of GaxIn1-xP solid solutions from computational alchemy. *Physical Review Letters*, **1994**, 72, 4001-4004	7.4	56
105	Temperature-dependent surface relaxations of Ag(111). *Physical Review B*, **1999**, 59, 970-974	3.3	53
104	Anomalous thermodynamic properties in ferropericlase throughout its spin crossover. *Physical Review B*, **2009**, 80,	3.3	52
103	Tuning the morphology of gold clusters by substrate doping. *Journal of the American Chemical Society*, **2011**, 133, 2801-3	16.4	51
102	Theory of the Anomalous Rayleigh Dispersion at H/W(110) Surfaces. *Physical Review Letters*, **1996**, 77, 2491-2494	7.4	50
101	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
100	Structural evolution of amino acid crystals under stress from a non-empirical density functional. *Journal of Physics Condensed Matter*, **2012**, 24, 424209	1.8	48
99	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
98	Interface mode in Si/Ge superlattices: Theory and experiments. *Physical Review B*, **1993**, 48, 8959-8962	3.3	48
97	First-principles study of the thermal expansion of Be(10$\bar{1}$0). *Physical Review B*, **2002**, 65,	3.3	47

96	Electron-phonon interaction at the Be(0001) surface. *Physical Review Letters*, **2003**, 91, 166803	7.4	44
95	Ab Initio Study of Be (0001) Surface Thermal Expansion. *Physical Review Letters*, **1998**, 81, 2096-2099	7.4	44
94	The Interaction of Ethylene with Perfect and Defective Ag(001) Surfaces. *Journal of Physical Chemistry B*, **2002**, 106, 9839-9846	3.4	43
93	Anisotropic thermal expansion in silicates: A density functional study of □eucryptite and related materials. *Physical Review B*, **2000**, 62, 11487-11493	3.3	43
92	Ab initio phonon calculations in solids. *Physica B: Condensed Matter*, **1996**, 219-220, 439-441	2.8	43
91	Ab initio 27Al NMR chemical shifts and quadrupolar parameters for Al2O3 phases and their precursors. *Physical Review B*, **2011**, 84,	3.3	42
90	Highly under-coordinated atoms at Rh surfaces: interplay of strain and coordination effects on core level shift. *New Journal of Physics*, **2007**, 9, 143-143	2.9	42
89	Adsorption of atomic oxygen on Ag(): a study based on density-functional theory. *Surface Science*, **2002**, 501, 182-190	1.8	42
88	The mechanism for the 3□ distortion of Sn/Ge(111). *Surface Science*, **2000**, 454-456, 172-177	1.8	41
87	Structural and Electronic Properties of a Wide-Gap Quaternary Solid Solution: (Zn, Mg) (S, Se). *Physical Review Letters*, **1998**, 80, 4939-4942	7.4	40
86	The reconstruction of Rh(001) upon oxygen adsorption. *Surface Science*, **1998**, 410, 151-157	1.8	38
85	Dipole-Quadrupole Interactions and the Nature of Phase III of Compressed Hydrogen. *Physical Review Letters*, **1999**, 83, 4097-4100	7.4	38
84	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
83	Core level shifts of undercoordinated Pt atoms. *Journal of Chemical Physics*, **2008**, 128, 114706	3.9	37
82	Infrared reflectivity by transverse-optical phonons in (GaAs)m/(AlAs)n ultrathin-layer superlattices. *Physical Review B*, **1991**, 43, 14754-14757	3.3	37
81	The reconstruction of nickel and rhodium (001) surfaces upon carbon, nitrogen or oxygen adsorptions. *Surface Science*, **1999**, 437, 18-28	1.8	36
80	Correlation energy within exact-exchange adiabatic connection fluctuation-dissipation theory: Systematic development and simple approximations. *Physical Review B*, **2014**, 90,	3.3	35
79	Anomalous pressure-induced transition(s) in ice XI. *Physical Review Letters*, **2004**, 92, 105502	7.4	35

78	Disproportionation phenomena on free and strained Sn/Ge(111) and Sn/Si(111) surfaces. *Physical Review Letters*, **2002**, 89, 126803	7.4	35
77	CO□Pt(111): GGA density functional study of site preference for adsorption. *Physical Review B*, **2008**, 77,	3.3	34
76	Adsorption of chlorine on Ag(111): No subsurface Cl at low coverage. *Physical Review B*, **2008**, 78,	3.3	33
75	Ab initio self-consistent total-energy calculations within the EXX/RPA formalism. *Physical Review B*, **2014**, 90,	3.3	32
74	First-principles study of vacancy formation and migration energies in tantalum. *Physical Review B*, **1999**, 60, 7001-7005	3.3	31
73	Order□isorder phase boundary between ice VII and VIII obtained by first principles. *Chemical Physics Letters*, **2010**, 499, 236-240	2.5	30
72	Structure and dynamics of oxygen adsorbed on Ag(100) vicinal surfaces. *Physical Review B*, **2004**, 69,	3.3	29
71	Nano-Scale Corrugations in Graphene: A Density Functional Theory Study of Structure, Electronic Properties and Hydrogenation. *Journal of Physical Chemistry C*, **2015**, 119, 7900-7910	3.8	28
70	Complete 13C NMR chemical shifts assignment for cholesterol crystals by combined CP-MAS spectral editing and ab initio GIPAW calculations with dispersion forces. *Journal of Physical Chemistry A*, **2012**, 116, 3765-9	2.8	27
69	Analysis of methane-to-methanol conversion on clean and defective Rh surfaces. *Journal of Chemical Physics*, **2006**, 125, 44701	3.9	27
68	Geometric and electronic structure of the N□Rh(100) system by core-level photoelectron spectroscopy: Experiment and theory. *Physical Review B*, **2006**, 74,	3.3	27
67	Ab-initio dynamical properties of the Be(0001) surface. *Surface Science*, **1998**, 402-404, 715-718	1.8	26
66	High-precision calculation of Hartree-Fock energy of crystals. *Journal of Computational Chemistry*, **2008**, 29, 2098-106	3.5	24
65	Beyond the random phase approximation with a local exchange vertex. *Physical Review B*, **2018**, 98,	3.3	23
64	Structural models of activated □alumina surfaces revisited: Thermodynamics, NMR and IR spectroscopies from ab initio calculations. *Chemical Physics*, **2013**, 423, 62-72	2.3	23
63	Enhanced Chemical Reactivity of Under-Coordinated Atoms at Pt□Rh Bimetallic Surfaces: A Spectroscopic Characterization. *Journal of Physical Chemistry C*, **2011**, 115, 3378-3384	3.8	23
62	Toward an accurate and efficient theory of physisorption. I. Development of an augmented density-functional theory model. *Journal of Physical Chemistry A*, **2008**, 112, 9993-1005	2.8	23
61	Interplay between bonding and magnetism in the binding of NO to Rh clusters. *Journal of Chemical Physics*, **2008**, 128, 194708	3.9	23

60	Surface structure and core-level shifts in lead chalcogenide (001) surfaces. *Physical Review B*, **2000**, 63,	3.3	23
59	Ag-Cu catalysts for ethylene epoxidation: selectivity and activity descriptors. *Journal of Chemical Physics*, **2013**, 138, 184707	3.9	20
58	Adsorption of ethylene on the Ag() surface. *Surface Science*, **2002**, 507-510, 62-68	1.8	20
57	Piezoelectricity in III-V and II-VI semiconductors: A systematic ab-initio calculation. *Ferroelectrics*, **1990**, 111, 19-22	0.6	20
56	Floating bonds and gap states in a-Si and a-Si:H from first principles calculations. *Europhysics Letters* , **1999**, 47, 481-486	1.6	19
55	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
54	Ab initio study of phonons in wurtzite AlxGa1□N alloys. *Applied Physics Letters*, **2000**, 76, 2101-2103	3.4	18
53	Nature of the Volume Isotope Effect in Ice. *Physical Review Letters*, **2015**, 115, 173005	7.4	17
52	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
51	Pressure induced high spin to low spin transition in magnesiow□stite. *Physica Status Solidi (B): Basic Research*, **2006**, 243, 2111-2116	1.3	17
50	Ab initio study of Be surface dynamical properties. *Surface Science*, **2000**, 454-456, 442-446	1.8	17
49	□Glycine: insight into the mechanism of a polymorphic phase transition. *IUCrJ*, **2017**, 4, 569-574	4.7	17
48	Molecular bonding with the RPAx: From weak dispersion forces to strong correlation. *Physical Review B*, **2016**, 93,	3.3	16
47	Subsurface Oxygen Stabilization by a Third Species: Carbonates on Ag(210). *Journal of Physical Chemistry C*, **2007**, 111, 10923-10930	3.8	15
46	Structure and dynamics of the missing-row reconstruction on O/Cu(001) and O/Ag(001). *Surface Science*, **2006**, 600, 5074-5079	1.8	15
45	Adsorption of ethylene on stepped Ag() surfaces. *Surface Science*, **2004**, 566-568, 1018-1023	1.8	15
44	On-surface and subsurface adsorption of oxygen on stepped Ag(210) and Ag(410) surfaces. *Surface Science*, **2004**, 566-568, 1107-1111	1.8	15
43	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

42	Hubbard-corrected density functional perturbation theory with ultrasoft pseudopotentials. *Physical Review B*, **2020**, 101,	3.3	14
41	Stability of Intermediate States for Ethylene Epoxidation on Ag□Cu Alloy Catalyst: A First-Principles Investigation. *Journal of Physical Chemistry C*, **2011**, 115, 10073-10079	3.8	14
40	The Ni3Al(111) surface structure: experiment and theory. *Journal of Physics Condensed Matter*, **2008**, 20, 195223	1.8	14
39	SixC1□O2 alloys: A possible route to stabilize carbon-based silica-like solids?. *Solid State Communications*, **2007**, 144, 273-276	1.6	14
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37	NO adsorption on Rh(100). I. Structural characterization of the adlayers. *Journal of Chemical Physics*, **2003**, 119, 12525-12533	3.9	14
36	Effects of disorder on the optical gap of (Zn,Mg)(S,Se). *Applied Physics Letters*, **1999**, 75, 2746-2748	3.4	13
35	Surface Core Level Shift: High Sensitive Probe to Oxygen-Induced Reconstruction of Rh(100). *Journal of Physical Chemistry C*, **2009**, 113, 13192-13198	3.8	12
34	Van der Waals coefficients of atoms and molecules from a simple approximation for the polarizability. *Physical Review B*, **2009**, 79,	3.3	12
33	The (1 X 1) --> hexagonal structural transition on Pt(100) studied by high-energy resolution core level photoemission. *Journal of Chemical Physics*, **2007**, 127, 164702	3.9	12
32	Phonons in nonlocal van der Waals density functional theory. *Physical Review B*, **2016**, 93,	3.3	11
31	Photoactivated processes in optical fibers: generation and conversion mechanisms of twofold coordinated Si and Ge atoms. *Nanotechnology*, **2017**, 28, 195202	3.4	10
30	Phonon Softening and Elastic Instabilities in the Cubic-to-Orthorhombic Structural Transition of CsH. *Physical Review Letters*, **1997**, 78, 4958-4961	7.4	10
29	On-surface and sub-surface oxygen adsorption on Ag(210): Vibrational properties. *Surface Science*, **2005**, 587, 50-54	1.8	10
28	Surface oscillatory thermal expansion: Mg(101□0). *Physical Review B*, **2001**, 63,	3.3	10
27	Role of defects in the electronic properties of amorphous/crystalline Si interface. *Physical Review B*, **2001**, 64,	3.3	10
26	Substrate doping: A strategy for enhancing reactivity on gold nanocatalysts by tuning sp bands. *Journal of Chemical Physics*, **2015**, 143, 144307	3.9	9
25	Effective coordination as a predictor of adsorption energies: A model study of NO on Rh(100) and Rh/MgO(100) surfaces. *Physical Review B*, **2009**, 79,	3.3	9

24	Finding Reaction Pathways and Transition States: r-ARTn and d-ARTn as an Efficient and Versatile Alternative to String Approaches. *Journal of Chemical Theory and Computation*, **2020**, 16, 6726-6734	6.4	9
23	Lithium Adsorption on Graphene at Finite Temperature. *Journal of Physical Chemistry C*, **2018**, 122, 20800-20808	3.7	8
22	Optical phonon probes of the lateral scale of interface roughness: A theoretical investigation. *Solid-State Electronics*, **1994**, 37, 621-624	1.7	8
21	Multilayer thermal expansion of Be(0001) determined from surface core level shifts. *Europhysics Letters*, **2003**, 64, 364-370	1.6	7
20	Vibrational properties of Si/Ge superlattices: Theory and in-plane Raman scattering experiments. *Solid-State Electronics*, **1994**, 37, 757-760	1.7	7
19	Experimental and Theoretical Surface Core Level Shift Study of the S-Rh(100) Local Environment. *Journal of Physical Chemistry C*, **2007**, 111, 4003-4013	3.8	6
18	Effective coordination number: A simple indicator of activation energies for NO dissociation on Rh(100) surfaces. *Physical Review B*, **2009**, 80,	3.3	5
17	Direct Methane-to-Methanol Conversion: Insight from First-Principles Calculations. *Journal of Physical Chemistry C*, **2007**, 111, 17015-17019	3.8	5
16	The CECAM electronic structure library and the modular software development paradigm. *Journal of Chemical Physics*, **2020**, 153, 024117	3.9	5
15	Compact atomic descriptors enable accurate predictions via linear models. *Journal of Chemical Physics*, **2021**, 154, 224112	3.9	5
14	A parallel orbital-updating based plane-wave basis method for electronic structure calculations. *Journal of Computational Physics*, **2017**, 348, 482-492	4.1	4
13	Data-driven simulation and characterisation of gold nanoparticle melting. *Nature Communications*, **2021**, 12, 6056	17.4	4
12	Coordination defects in amorphous silicon and hydrogenated amorphous silicon: a characterization from first-principles calculations. *The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties*, **2000**, 80, 515-521		3
11	Collective dipole effects in ionic transport under electric fields. *Nature Communications*, **2020**, 11, 3330	17.4	3
10	A systematic approach to generating accurate neural network potentials: the case of carbon. *Npj Computational Materials*, **2021**, 7,	10.9	3
9	v-PO micro-clustering in P-doped silica studied by a first-principles Raman investigation. *Scientific Reports*, **2019**, 9, 7126	4.9	2
8	Publisher's Note: Anomalous thermodynamic properties in ferropericlase throughout its spin crossover [Phys. Rev. B 80, 014409 (2009)]. *Physical Review B*, **2009**, 80,	3.3	2
7	Structural and elastic properties of strained Mg1−xSrxSe revealed. *Solid State Communications*, **2014**, 178, 46-49	1.6	1

6	Vacancy Properties In 5d Bcc Transition Metals: Ab Initio Study At Finite Electron Temperature. *Materials Research Society Symposia Proceedings*, **1997**, 481, 189		1
5	Ab Initio Calculation of Phonon Spectra in Semiconductors: from Pure Crystals to Alloys and Superlattices **1993**, 243-277		1
4	Exchange-correlation errors at harmonic and anharmonic orders: the case of bulk Cu. *Bulletin of Materials Science*, **2003**, 26, 75-78	1.7	0
3	ActivationRelaxation Technique: An efficient way to find minima and saddle points of potential energy surfaces. *Computational Materials Science*, **2022**, 209, 111363	3.2	0
2	Structure and Energetics of Vacancies in Body Centered Cubic Hafnium under Pressure: First-Principles Study. *Defect and Diffusion Forum*, **2001**, 194-199, 295-302	0.7	
1	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	