Stefano de Gironcoli

List of Publications by Year
in descending order

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154 papers	45,093 citations	36271 51 h-index	8384 147 g-index
155 all docs	155 docs citations	155 times ranked	31788 citing authors

#	Article	IF	Citations
1	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502.	0.7	18,183
2	Phonons and related crystal properties from density-functional perturbation theory. Reviews of Modern Physics, 2001, 73, 515-562.	16.4	7,534
3	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	0.7	4,303
4	Linear response approach to the calculation of the effective interaction parameters in theLDA+Umethod. Physical Review B, 2005, 71, .	1.1	2,754
5	Ab initiocalculation of phonon dispersions in semiconductors. Physical Review B, 1991, 43, 7231-7242.	1.1	1,619
6	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
7	Q<scp>uantum</scp> ESPRESSO toward the exascale. Journal of Chemical Physics, 2020, 152, 154105.	1.2	796
8	Hubbard-corrected DFT energy functionals: The LDA+U description of correlated systems. International Journal of Quantum Chemistry, 2014, 114, 14-49.	1.0	533
9	Nonlocal van der Waals density functional made simple and efficient. Physical Review B, 2013, 87, .	1.1	471
10	Taming multiple valency with density functionals:â€ƒA case study of defective ceria. Physical Review B, 2005, 71, .	1.1	383
11	Electronic and Atomistic Structures of Clean and Reduced Ceria Surfaces. Journal of Physical Chemistry B, 2005, 109, 22860-22867.	1.2	358
12	Lattice dynamics of metals from density-functional perturbation theory. Physical Review B, 1995, 51, 6773-6776.	1.1	283
13	High-pressure lattice dynamics and thermoelasticity of MgO. Physical Review B, 2000, 61, 8793-8800.	1.1	278
14	Spin Transition in MagnesiowÃ¼stite in Earthâ€™s Lower Mantle. Physical Review Letters, 2006, 96, 198501.	2.9	257
15	First-Principles Determination of Elastic Anisotropy and Wave Velocities of MgO at Lower Mantle Conditions. Science, 1999, 286, 1705-1707.	6.0	236
16	Ab initiocalculation of phonon dispersions in II-VI semiconductors. Physical Review B, 1993, 47, 3588-3592.	1.1	229
17	Piezoelectric properties of III-V semiconductors from first-principles linear-response theory. Physical Review Letters, 1989, 62, 2853-2856.	2.9	221
18	Thermoelastic Properties ofMgSiO3-Perovskite: Insights on the Nature of the Earthâ€™s Lower Mantle. Physical Review Letters, 2004, 92, 018501.	2.9	210

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19	First-principles codes for computational crystallography in the Quantum-ESPRESSO package. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.4	177
20	Reply to â€œComment on â€˜Taming multiple valency with density functionals: A case study of defective ceria' â€• Physical Review B, 2005, 72, .	1.1	177
21	Structure and thermodynamics ofSixGe1â^'xalloys fromab initioMonte Carlo simulations. Physical Review Letters, 1991, 66, 2116-2119.	2.9	155
22	Ab initiolattice dynamics ofMgSiO3perovskite at high pressure. Physical Review B, 2000, 62, 14750-14756.	1.1	134
23	Templated Growth of Metal-Organic Coordination Chains at Surfaces. Angewandte Chemie - International Edition, 2005, 44, 6142-6145.	7.2	125
24	First-principles calculation of the thermal properties of silver. Physical Review B, 1999, 59, 965-969.	1.1	124
25	Efficient calculation of exact exchange and RPA correlation energies in the adiabatic-connection fluctuation-dissipation theory. Physical Review B, 2009, 79, .	1.1	120
26	Hydrogen and Coordination Bonding Supramolecular Structures of Trimesic Acid on Cu(110). Journal of Physical Chemistry A, 2007, 111, 12589-12603.	1.1	118
27	Phonon dispersions inGaxAl1â^'xAs alloys. Physical Review Letters, 1990, 65, 84-87.	2.9	108
28	Î±â†”Î² phase transition in tin: A theoretical study based on density-functional perturbation theory. Physical Review B, 1998, 57, 10421-10423.	1.1	106
29	Ab initiocalculation of the thermal properties of Cu:â€ƒPerformance of the LDA and GGA. Physical Review B, 2002, 65, .	1.1	103
30	Phonons in Si-Ge systems: Anab initiointeratomic-force-constant approach. Physical Review B, 1992, 46, 2412-2419.	1.1	90
31	Effects of disorder on the Raman spectra of GaAs/AlAs superlattices. Physical Review B, 1992, 45, 4280-4288.	1.1	88
32	Interaction of Hydrogen with Cerium Oxide Surfaces:â€‰ a Quantum Mechanical Computational Study. Journal of Physical Chemistry B, 2006, 110, 19380-19385.	1.2	85
33	High-pressure thermal expansion, bulk modulus, and phonon structure of diamond. Physical Review B, 1999, 60, 9444-9449.	1.1	84
34	Ab initiophonon dispersions of Fe and Ni. Physical Review B, 2000, 62, 273-277.	1.1	84
35	Vibrational properties of MnO and NiO from DFT<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mo>+</mml:mo><mml:mspace width="0.28em" /><mml:mi>U</mml:mi></mml:mrow></mml:math>-based density functional perturbation theory. Physical Review B, 2011, 84, .	1.1	82
36	Engineering the Reactivity of Metal Catalysts:Â A Model Study of Methane Dehydrogenation on Rh(111). Journal of the American Chemical Society, 2004, 126, 16732-16733.	6.6	80

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37	Structural, electronic, and magnetic properties ofFe2SiO4fayalite: Comparison of LDA and GGA results. Physical Review B, 2003, 67, .	1.1	75
38	Vacancy self-diffusion parameters in tungsten: Finite electron-temperature LDA calculations. Physical Review B, 1998, 57, 11184-11192.	1.1	74
39	Successful a Priori Modeling of CO Adsorption on Pt(111) Using Periodic Hybrid Density Functional Theory. Journal of the American Chemical Society, 2007, 129, 10402-10407.	6.6	73
40	In-plane Raman scattering of (001)-Si/Ge superlattices: Theory and experiment. Physical Review B, 1994, 49, 5406-5414.	1.1	71
41	Anomalous thermodynamic properties in ferropericlase throughout its spin crossover. Physical Review B, 2009, 80, .	1.1	68
42	Isobaric first-principles molecular dynamics of liquid water with nonlocal van der Waals interactions. Journal of Chemical Physics, 2015, 142, 034501.	1.2	68
43	Phonon Softening and Superconductivity in Tellurium under Pressure. Physical Review Letters, 1996, 77, 1151-1154.	2.9	67
44	What determines the catalyst's selectivity in the ethylene epoxidation reaction. Journal of Catalysis, 2008, 254, 304-309.	3.1	67
45	Structural evolution of amino acid crystals under stress from a non-empirical density functional. Journal of Physics Condensed Matter, 2012, 24, 424209.	0.7	65
46	Structure and phase stability ofGaxIn1âˆ’xP solid solutions from computational alchemy. Physical Review Letters, 1994, 72, 4001-4004.	2.9	61
47	Methane Dehydrogenation on Rh@Cu(111):Â A First-Principles Study of a Model Catalyst. Journal of the American Chemical Society, 2006, 128, 12448-12454.	6.6	60
48	Temperature-dependent surface relaxations of Ag(111). Physical Review B, 1999, 59, 970-974.	1.1	58
49	Tuning the Morphology of Gold Clusters by Substrate Doping. Journal of the American Chemical Society, 2011, 133, 2801-2803.	6.6	56
50	Piezoelectricity in III-V and II-VI semiconductors: A systematic ab-initio calculation. Ferroelectrics, 1990, 111, 19-22.	0.3	55
51	First principles thermoelasticity of MgSiO3-perovskite: Consequences for the inferred properties of the lower mantle. Geophysical Research Letters, 2001, 28, 2699-2702.	1.5	55
52	Anisotropic thermal expansion in silicates: A density functional study ofÎ²-eucryptite and related materials. Physical Review B, 2000, 62, 11487-11493.	1.1	53
53	First-principles study of the thermal expansion ofBe(101Â¯0). Physical Review B, 2002, 65, .	1.1	52
54	Theory of the Anomalous Rayleigh Dispersion at H/W(110) Surfaces. Physical Review Letters, 1996, 77, 2491-2494.	2.9	51

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55	Ab initio phonon calculations in solids. Physica B: Condensed Matter, 1996, 219-220, 439-441.	1.3	51
56	Effects of disorder on the vibrational properties of SiGe alloys: Failure of mean-field approximations. Physical Review Letters, 1992, 69, 1959-1962.	2.9	49
57	Interface mode in Si/Ge superlattices: Theory and experiments. Physical Review B, 1993, 48, 8959-8962.	1.1	48
58	Electron-Phonon Interaction at the Be(0001) Surface. Physical Review Letters, 2003, 91, 166803.	2.9	48
59	Ab initio<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mrow /><mml:mn>27</mml:mn></mml:msup></mml:math>Al NMR chemical shifts and quadrupolar parameters for Al<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>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow />	1.1	48
60	Adsorption of atomic oxygen on Ag(): a study based on density-functional theory. Surface Science, 2002, 501, 182-190.	0.8	47
61	Ab Initio Study of Be (0001) Surface Thermal Expansion. Physical Review Letters, 1998, 81, 2096-2099.	2.9	46
62	Dipole-Quadrupole Interactions and the Nature of Phase III of Compressed Hydrogen. Physical Review Letters, 1999, 83, 4097-4100.	2.9	46
63	The Interaction of Ethylene with Perfect and Defective Ag(001) Surfaces. Journal of Physical Chemistry B, 2002, 106, 9839-9846.	1.2	45
64	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.	1.2	45
65	Structural and Electronic Properties of a Wide-Gap Quaternary Solid Solution: (Zn, Mg) (S, Se). Physical Review Letters, 1998, 80, 4939-4942.	2.9	43
66	The mechanism for the 3Ã—3 distortion of Sn/Ge(111). Surface Science, 2000, 454-456, 172-177.	0.8	43
67	Hubbard-corrected density functional perturbation theory with ultrasoft pseudopotentials. Physical Review B, 2020, 101, .	1.1	43
68	The reconstruction of Rh(001) upon oxygen adsorption. Surface Science, 1998, 410, 151-157.	0.8	41
69	Core level shifts of undercoordinated Pt atoms. Journal of Chemical Physics, 2008, 128, 114706.	1.2	41
70	Correlation energy within exact-exchange adiabatic connection fluctuation-dissipation theory: Systematic development and simple approximations. Physical Review B, 2014, 90, .	1.1	41
71	Orderâ€“disorder phase boundary between ice VII and VIII obtained by first principles. Chemical Physics Letters, 2010, 499, 236-240.	1.2	40
72	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.	1.5	39

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73	Infrared reflectivity by transverse-optical phonons in (GaAs)m/(AlAs)nultrathin-layer superlattices. Physical Review B, 1991, 43, 14754-14757.	1.1	38
74	Anomalous Pressure-Induced Transition(s) in Ice XI. Physical Review Letters, 2004, 92, 105502.	2.9	37
75	Adsorption of chlorine on Ag(111): No subsurface Cl at low coverage. Physical Review B, 2008, 78, .	1.1	37
76	First-principles study of vacancy formation and migration energies in tantalum. Physical Review B, 1999, 60, 7001-7005.	1.1	36
77	The reconstruction of nickel and rhodium (001) surfaces upon carbon, nitrogen or oxygen adsorptions. Surface Science, 1999, 437, 18-28.	0.8	36
78	Disproportionation Phenomena on Free and StrainedSn/Ge(111)andSn/Si(111)Surfaces. Physical Review Letters, 2002, 89, 126803.	2.9	36
79	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:mi mathvariant="normal">O</mml:mi><mml:mo>âˆ•</mml:mo><mml:mi mathvariant="normal">Pt</mml:mi><mml:mrow><mml:mo>(</mml:mo><mml:mn>111</mml:mn><mml:mo>)</mml:mo></mml:mrow> GGA density functional study of site preference for adsorption. Physical Review B, 2008, 77, .	1.1	36
80	Ab initioself-consistent total-energy calculations within the EXX/RPA formalism. Physical Review B, 2014, 90, .	1.1	35
81	Structure and dynamics of oxygen adsorbed on Ag(100) vicinal surfaces. Physical Review B, 2004, 69, .	1.1	32
82	Analysis of methane-to-methanol conversion on clean and defective Rh surfaces. Journal of Chemical Physics, 2006, 125, 044701.	1.2	31
83	Beyond the random phase approximation with a local exchange vertex. Physical Review B, 2018, 98, .	1.1	31
84	Geometric and electronic structure of theNâˆ•Rh(100)system by core-level photoelectron spectroscopy: Experiment and theory. Physical Review B, 2006, 74, .	1.1	29
85	Structural models of activated Î³-alumina surfaces revisited: Thermodynamics, NMR and IR spectroscopies from ab initio calculations. Chemical Physics, 2013, 423, 62-72.	0.9	29
86	Data-driven simulation and characterisation of gold nanoparticle melting. Nature Communications, 2021, 12, 6056.	5.8	29
87	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, 3765-3769.	1.1	28
88	Ab-initio dynamical properties of the Be(0001) surface. Surface Science, 1998, 402-404, 715-718.	0.8	26
89	Surface structure and core-level shifts in lead chalcogenide (001) surfaces. Physical Review B, 2000, 63, .	1.1	26
90	Highâ€precision calculation of Hartreeâ€Fock energy of crystals. Journal of Computational Chemistry, 2008, 29, 2098-2106.	1.5	25

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91	Interplay between bonding and magnetism in the binding of NO to Rh clusters. Journal of Chemical Physics, 2008, 128, 194708.	1.2	25
92	Ag-Cu catalysts for ethylene epoxidation: Selectivity and activity descriptors. Journal of Chemical Physics, 2013, 138, 184707.	1.2	25
93	Toward an Accurate and Efficient Theory of Physisorption. I. Development of an Augmented Density-Functional Theory Model. Journal of Physical Chemistry A, 2008, 112, 9993-10005.	1.1	24
94	Enhanced Chemical Reactivity of Under-Coordinated Atoms at Ptâ˜Rh Bimetallic Surfaces: A Spectroscopic Characterization. Journal of Physical Chemistry C, 2011, 115, 3378-3384.	1.5	24
95	Adsorption of ethylene on the Ag() surface. Surface Science, 2002, 507-510, 62-68.	0.8	23
96	A systematic approach to generating accurate neural network potentials: the case of carbon. Npj Computational Materials, 2021, 7, .	3.5	23
97	Î¶-Glycine: insight into the mechanism of a polymorphic phase transition. IUCrJ, 2017, 4, 569-574.	1.0	23
98	Nature of the Volume Isotope Effect in Ice. Physical Review Letters, 2015, 115, 173005.	2.9	22
99	Ab initio study of phonons in wurtzite AlxGa1â˜xN alloys. Applied Physics Letters, 2000, 76, 2101-2103.	1.5	21
100	Activated Adsorption of Ethylene on Atomic-Oxygen-Covered Ag(100) and Ag(210):â€‰ Formation of an Oxametallacycle. Journal of Physical Chemistry C, 2008, 112, 1019-1027.	1.5	21
101	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.	2.3	21
102	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.	0.6	20
103	DFT Study of a Weakly Ï€-Bonded C2H4on Oxygen-Covered Ag(100). Journal of Physical Chemistry B, 2006, 110, 367-376.	1.2	20
104	Floating bonds and gap states in a-Si and a-Si:H from first principles calculations. Europhysics Letters, 1999, 47, 481-486.	0.7	19
105	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	1.2	19
106	Pressure induced high spin to low spin transition in magnesiowÃ¼stite. Physica Status Solidi (B): Basic Research, 2006, 243, 2111-2116.	0.7	18
107	Molecular bonding with the RPAx: From weak dispersion forces to strong correlation. Physical Review B, 2016, 93, .	1.1	18
108	Ab initio study of Be surface dynamical properties. Surface Science, 2000, 454-456, 442-446.	0.8	17

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109	Phonons in nonlocal van der Waals density functional theory. Physical Review B, 2016, 93, .	1.1	17
110	NO adsorption on Rh(100). I. Structural characterization of the adlayers. Journal of Chemical Physics, 2003, 119, 12525-12533.	1.2	16
111	Adsorption of ethylene on stepped Ag() surfaces. Surface Science, 2004, 566-568, 1018-1023.	0.8	16
112	SixC1â˜'xO2 alloys: A possible route to stabilize carbon-based silica-like solids?. Solid State Communications, 2007, 144, 273-276.	0.9	16
113	Subsurface Oxygen Stabilization by a Third Species:â€‰ Carbonates on Ag(210). Journal of Physical Chemistry C, 2007, 111, 10923-10930.	1.5	16
114	Compact atomic descriptors enable accurate predictions via linear models. Journal of Chemical Physics, 2021, 154, 224112.	1.2	16
115	On-surface and subsurface adsorption of oxygen on stepped Ag(210) and Ag(410) surfaces. Surface Science, 2004, 566-568, 1107-1111.	0.8	15
116	Structure and dynamics of the missing-row reconstruction on O/Cu(001) and O/Ag(001). Surface Science, 2006, 600, 5074-5079.	0.8	15
117	The Ni₃Al(111) surface structure: experiment and theory. Journal of Physics Condensed Matter, 2008, 20, 195223.	0.7	15
118	Stability of Intermediate States for Ethylene Epoxidation on Agâ€“Cu Alloy Catalyst: A First-Principles Investigation. Journal of Physical Chemistry C, 2011, 115, 10073-10079.	1.5	15
119	Photoactivated processes in optical fibers: generation and conversion mechanisms of twofold coordinated Si and Ge atoms. Nanotechnology, 2017, 28, 195202.	1.3	15
120	Effects of disorder on the optical gap of (Zn,Mg)(S,Se). Applied Physics Letters, 1999, 75, 2746-2748.	1.5	14
121	Surface oscillatory thermal expansion:â€ƒMg(101Â¯0). Physical Review B, 2001, 63, .	1.1	14
122	Co-adsorption of ethylene and oxygen on the Ag(001) surface. Surface Science, 2003, 532-535, 191-197.	0.8	14
123	Van der Waals coefficients of atoms and molecules from a simple approximation for the polarizability. Physical Review B, 2009, 79, .	1.1	14
124	On-surface and sub-surface oxygen adsorption on Ag(210): Vibrational properties. Surface Science, 2005, 587, 50-54.	0.8	12
125	The (1Ã—1)â†'hexagonal structural transition on Pt(100) studied by high-energy resolution core level photoemission. Journal of Chemical Physics, 2007, 127, 164702.	1.2	12
126	Surface Core Level Shift: High Sensitive Probe to Oxygen-Induced Reconstruction of Rh(100). Journal of Physical Chemistry C, 2009, 113, 13192-13198.	1.5	12

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127	Phonon Softening and Elastic Instabilities in the Cubic-to-Orthorhombic Structural Transition of CsH. Physical Review Letters, 1997, 78, 4958-4961.	2.9	11
128	Role of defects in the electronic properties of amorphous/crystalline Si interface. Physical Review B, 2001, 64, .	1.1	11
129	Lithium Adsorption on Graphene at Finite Temperature. Journal of Physical Chemistry C, 2018, 122, 20800-20808.	1.5	11
130	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, .	1.1	10
131	Direct Methane-to-Methanol Conversion:â€‰ Insight from First-Principles Calculations. Journal of Physical Chemistry C, 2007, 111, 17015-17019.	1.5	9
132	Substrate doping: A strategy for enhancing reactivity on gold nanocatalysts by tuning sp bands. Journal of Chemical Physics, 2015, 143, 144307.	1.2	9
133	Optical phonon probes of the lateral scale of interface roughness: A theoretical investigation. Solid-State Electronics, 1994, 37, 621-624.	0.8	8
134	Vibrational properties of Si/Ge superlattices: Theory and in-plane Raman scattering experiments. Solid-State Electronics, 1994, 37, 757-760.	0.8	7
135	Multilayer thermal expansion of Be(0001) determined from surface core level shifts. Europhysics Letters, 2003, 64, 364-370.	0.7	7
136	Experimental and Theoretical Surface Core Level Shift Study of the S-Rh(100) Local Environment. Journal of Physical Chemistry C, 2007, 111, 4003-4013.	1.5	7
137	v-P2O5 micro-clustering in P-doped silica studied by a first-principles Raman investigation. Scientific Reports, 2019, 9, 7126.	1.6	7
138	Effective coordination number: A simple indicator of activation energies for NO dissociation on Rh(100) surfaces. Physical Review B, 2009, 80, .	1.1	6
139	Collective dipole effects in ionic transport under electric fields. Nature Communications, 2020, 11, 3330.	5.8	6
140	A parallel orbital-updating based plane-wave basis method for electronic structure calculations. Journal of Computational Physics, 2017, 348, 482-492.	1.9	5
141	Activationâ€“Relaxation Technique: An efficient way to find minima and saddle points of potential energy surfaces. Computational Materials Science, 2022, 209, 111363.	1.4	5
142	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.	0.6	3
143	Publisher's Note: Anomalous thermodynamic properties in ferropericlase throughout its spin crossover [Phys. Rev. B80, 014409 (2009)]. Physical Review B, 2009, 80, .	1.1	3
144	Clusters of Defects as a Possible Origin of Random Telegraph Signal in Imager Devices: a DFT based Study. , 2021, , .		3

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145	Ab Initio Calculation of Phonon Spectra in Semiconductors: from Pure Crystals to Alloys and Superlattices. , 1993, , 243-277.		1
146	Vacancy Properties In 5d Bcc Transition Metals: Ab Initio Study At Finite Electron Temperature. Materials Research Society Symposia Proceedings, 1997, 481, 189.	0.1	1
147	Exchange-correlation errors at harmonic and anharmonic orders: the case of bulk Cu. Bulletin of Materials Science, 2003, 26, 75-78.	0.8	1
148	Structural and elastic properties of strained Mg1âˆ’xSrxSe revealed. Solid State Communications, 2014, 178, 46-49.	0.9	1
149	First-principles characterization of Mg low-index surfaces: Structure, reconstructions, and surface core-level shifts. Physical Review B, 2019, 100, .	1.1	1
150	Defect creation and Diffusion under electric fields from first-principles: the prototypical case of silicon dioxide. , 2019, , .		1
151	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.	3.1	0
152	Structure and Energetics of Vacancies in Body Centered Cubic Hafnium under Pressure: First-Principles Study. Defect and Diffusion Forum, 2001, 194-199, 295-302.	0.4	0
153	Publisher's Note: Molecular bonding with the RPAx: From weak dispersion forces to strong correlation [Phys. Rev. B 93, 195108 (2016)]. Physical Review B, 2016, 93, .	1.1	0
154	Developing a Neural Network potential to investigate interface phenomena in solid-phase epitaxy. , 2021, , .		0