Francesco Mauri

List of Publications by Year
in descending order

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288 papers	63,434 citations	4388 86 h-index	767 249 g-index
293 all docs	293 docs citations	293 times ranked	51620 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.	1.8	18,183
2	Raman Spectrum of Graphene and Graphene Layers. Physical Review Letters, 2006, 97, 187401.	7.8	12,689
3	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	1.8	4,303
4	All-electron magnetic response with pseudopotentials: NMR chemical shifts. Physical Review B, 2001, 63, .	3.2	1,502
5	Breakdown of the adiabatic Bornâ€“Oppenheimer approximation in graphene. Nature Materials, 2007, 6, 198-201.	27.5	1,229
6	Calculation of NMR chemical shifts for extended systems using ultrasoft pseudopotentials. Physical Review B, 2007, 76, .	3.2	794
7	Kohn Anomalies and Electron-Phonon Interactions in Graphite. Physical Review Letters, 2004, 93, 185503.	7.8	779
8	Structure, Stability, Edge States, and Aromaticity of Graphene Ribbons. Physical Review Letters, 2008, 101, 096402.	7.8	582
9	Nonadiabatic Kohn Anomaly in a Doped Graphene Monolayer. Physical Review Letters, 2006, 97, 266407.	7.8	477
10	Theory of double-resonant Raman spectra in graphene: Intensity and line shape of defect-induced and two-phonon bands. Physical Review B, 2011, 84, .	3.2	476
11	Thermal Conductivity of Graphene and Graphite: Collective Excitations and Mean Free Paths. Nano Letters, 2014, 14, 6109-6114.	9.1	449
12	First-Principles Calculation of NMR Parameters Using the Gauge Including Projector Augmented Wave Method: A Chemistâ€™s Point of View. Chemical Reviews, 2012, 112, 5733-5779.	47.7	446
13	Orbital formulation for electronic-structure calculations with linear system-size scaling. Physical Review B, 1993, 47, 9973-9976.	3.2	436
14	Phonon-mediated superconductivity in graphene by lithium deposition. Nature Physics, 2012, 8, 131-134.	16.7	431
15	Optical phonons in carbon nanotubes: Kohn anomalies, Peierls distortions, and dynamic effects. Physical Review B, 2007, 75, .	3.2	418
16	Two-Dimensional Self-Assembly of Supramolecular Clusters and Chains. Physical Review Letters, 1999, 83, 324-327.	7.8	396
17	Phonon Anharmonicities in Graphite and Graphene. Physical Review Letters, 2007, 99, 176802.	7.8	391
18	Accurate First Principles Prediction of17O NMR Parameters in SiO2:Â Assignment of the Zeolite Ferrierite Spectrum. Journal of the American Chemical Society, 2003, 125, 541-548.	13.7	389

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19	Phonon hydrodynamics in two-dimensional materials. Nature Communications, 2015, 6, 6400.	12.8	385
20	High-Pressure Hydrogen Sulfide from First Principles: A Strongly Anharmonic Phonon-Mediated Superconductor. Physical Review Letters, 2015, 114, 157004.	7.8	377
21	Raman spectroscopy as probe of nanometre-scale strain variations in graphene. Nature Communications, 2015, 6, 8429.	12.8	341
22	Phonon linewidths and electron-phonon coupling in graphite and nanotubes. Physical Review B, 2006, 73, .	3.2	335
23	First-Principles Calculation of Vibrational Raman Spectra in Large Systems: Signature of Small Rings in CrystallineSiO2. Physical Review Letters, 2003, 90, 036401.	7.8	313
24	Ab InitioTheory of NMR Chemical Shifts in Solids and Liquids. Physical Review Letters, 1996, 77, 5300-5303.	7.8	311
25	Magnesium incorporation into hydroxyapatite. Biomaterials, 2011, 32, 1826-1837.	11.4	296
26	X-ray absorption near-edge structure calculations with the pseudopotentials: Application to theKedge in diamond andÎ±-quartz. Physical Review B, 2002, 66, .	3.2	281
27	Anharmonic free energies and phonon dispersions from the stochastic self-consistent harmonic approximation: Application to platinum and palladium hydrides. Physical Review B, 2014, 89, .	3.2	264
28	Impact of the electron-electron correlation on phonon dispersion: Failure of LDA and GGA DFT functionals in graphene and graphite. Physical Review B, 2008, 78, .	3.2	257
29	Unified theory of thermal transport in crystals and glasses. Nature Physics, 2019, 15, 809-813.	16.7	255
30	Electron Transport and Hot Phonons in Carbon Nanotubes. Physical Review Letters, 2005, 95, 236802.	7.8	250
31	Total-energy global optimizations using nonorthogonal localized orbitals. Physical Review B, 1995, 52, 1640-1648.	3.2	247
32	Theoretical Explanation of Superconductivity inC6Ca. Physical Review Letters, 2005, 95, 237002.	7.8	223
33	Ab Initio Study of the Hydroxylated Surface of Amorphous Silica: A Representative Model. Chemistry of Materials, 2008, 20, 3336-3344.	6.7	222
34	Quantum hydrogen-bond symmetrization in the superconducting hydrogen sulfide system. Nature, 2016, 532, 81-84.	27.8	222
35	Clarâ€™s Theory, Ï€-Electron Distribution, and Geometry of Graphene Nanoribbons. Journal of the American Chemical Society, 2010, 132, 3440-3451.	13.7	219
36	First-principles modeling of the infrared spectrum of kaolinite. American Mineralogist, 2001, 86, 1321-1330.	1.9	201

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37	Ab initiovariational approach for evaluating lattice thermal conductivity. Physical Review B, 2013, 88, .	3.2	199
38	Density functional perturbation theory for gated two-dimensional heterostructures: Theoretical developments and application to flexural phonons in graphene. Physical Review B, 2017, 96, .	3.2	198
39	Anomalous Highâ€Temperature Superconductivity in YH₆. Advanced Materials, 2021, 33, e2006832.	21.0	196
40	Quantum crystal structure in the 250-kelvin superconducting lanthanum hydride. Nature, 2020, 578, 66-69.	27.8	193
41	Electron-phonon coupling and electron self-energy in electron-doped graphene: Calculation of angular-resolved photoemission spectra. Physical Review B, 2007, 76, .	3.2	188
42	Transport Properties of Graphene in the High-Current Limit. Physical Review Letters, 2009, 103, 076601.	7.8	188
43	An Investigation of Weak CHÂ·Â·Â·O Hydrogen Bonds in Maltose Anomers by a Combination of Calculation and Experimental Solid-State NMR Spectroscopy. Journal of the American Chemical Society, 2005, 127, 10216-10220.	13.7	185
44	Effect of dimensionality on the charge-density wave in few-layer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>2</mml:mn><mml:msub><mml:mrow><mml:mi>H</mml:mi><mml:mtext>-NbSe</mml:mtext></mml:mrow> Physical Review B, 2009, 80, .	3.2	184
45	Equilibrium isotopic fractionation in the kaolinite, quartz, water system: Prediction from first-principles density-functional theory. Geochimica Et Cosmochimica Acta, 2007, 71, 3170-3181.	3.9	180
46	Anharmonic properties from a generalized third-orderab initioapproach: Theory and applications to graphite and graphene. Physical Review B, 2013, 87, .	3.2	180
47	Electronic-structure calculations and molecular-dynamics simulations with linear system-size scaling. Physical Review B, 1994, 50, 4316-4326.	3.2	176
48	First-Principles Calculation of 17O, 29Si, and 23Na NMR Spectra of Sodium Silicate Crystals and Glasses. Journal of Physical Chemistry B, 2004, 108, 4147-4161.	2.6	174
49	Iron isotope fractionation between pyrite (FeS2), hematite (Fe2O3) and siderite (FeCO3): A first-principles density functional theory study. Geochimica Et Cosmochimica Acta, 2009, 73, 6565-6578.	3.9	173
50	First-Principles Theory of Anharmonicity and the Inverse Isotope Effect in Superconducting Palladium-Hydride Compounds. Physical Review Letters, 2013, 111, 177002.	7.8	173
51	Variations in the work function of doped single- and few-layer graphene assessed by Kelvin probe force microscopy and density functional theory. Physical Review B, 2011, 83, .	3.2	170
52	Combined First-Principles Computational and Experimental Multinuclear Solid-State NMR Investigation of Amino Acids. Journal of Physical Chemistry A, 2005, 109, 6960-6969.	2.5	169
53	Si-O-Si bond-angle distribution in vitreous silica from first-principles29SiNMR analysis. Physical Review B, 2000, 62, R4786-R4789.	3.2	167
54	Acceleration schemes forab initiomolecular-dynamics simulations and electronic-structure calculations. Physical Review B, 1994, 50, 10561-10573.	3.2	165

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55	Charge-Density Wave and Superconducting Dome in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>TiSe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>from Electron-Phonon Interaction. Physical Review Letters, 2011, 106, 196406.	7.8	159
56	Two-dimensional FrÃ¶hlich interaction in transition-metal dichalcogenide monolayers: Theoretical modeling and first-principles calculations. Physical Review B, 2016, 94, .	3.2	155
57	First-principles calculations of x-ray absorption in a scheme based on ultrasoft pseudopotentials: From<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-quartz to high-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>T</mml:mi><mml:mi>c</mml:mi></mml:msub></mml:mrow></mml:math>com Physical Review B, 2009, 80, .	3.2	150
58	Electronâ€“Phonon Interactions and the Intrinsic Electrical Resistivity of Graphene. Nano Letters, 2014, 14, 1113-1119.	9.1	149
59	A comparison of methods for the calculation of NMR chemical shifts. Journal of Chemical Physics, 1999, 111, 1815-1822.	3.0	147
60	Ab initiostudy of gap opening and screening effects in gated bilayer graphene. Physical Review B, 2009, 79, .	3.2	147
61	Atomic Structure of IcosahedralB4CBoron Carbide from a First Principles Analysis of NMR Spectra. Physical Review Letters, 2001, 87, 085506.	7.8	145
62	First-Principles Theory of the EPRgTensor in Solids: Defects in Quartz. Physical Review Letters, 2002, 88, 086403.	7.8	139
63	Phonon Dispersion and Lifetimes inMgB2. Physical Review Letters, 2003, 90, 095506.	7.8	139
64	A combined first principles computational and solid-state NMR study of a molecular crystal: flurbiprofen. Physical Chemistry Chemical Physics, 2005, 7, 1402.	2.8	136
65	Doping in Carbon Nanotubes Probed by Raman and Transport Measurements. Physical Review Letters, 2007, 99, 136803.	7.8	135
66	Boroxol Rings in Liquid and Vitreous<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>from First Principles. Physical Review Letters, 2008, 101, 065504.	7.8	131
67	Structural control over equilibrium silicon and oxygen isotopic fractionation: A first-principles density-functional theory study. Chemical Geology, 2009, 258, 28-37.	3.3	128
68	First-principles theory of field-effect doping in transition-metal dichalcogenides: Structural properties, electronic structure, Hall coefficient, and electrical conductivity. Physical Review B, 2015, 91, .	3.2	127
69	Breakdown of Optical Phononsâ€™ Splitting in Two-Dimensional Materials. Nano Letters, 2017, 17, 3758-3763.	9.1	127
70	Wannier interpolation of the electron-phonon matrix elements in polar semiconductors: Polar-optical coupling in GaAs. Physical Review B, 2015, 92, .	3.2	126
71	Wannier and Bloch orbital computation of the nonlinear susceptibility. Physical Review B, 1994, 50, 5756-5759.	3.2	121
72	Dissociation products and structures of solid<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">S</mml:mi></mml:math>at strong compression. Physical Review B, 2016, 93, .	3.2	119

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73	Coupled dynamics of electrons and phonons in metallic nanotubes: Current saturation from hot-phonon generation. Physical Review B, 2006, 73, .	3.2	116
74	First-principles study of the OH-stretching modes of gibbsite. American Mineralogist, 2006, 91, 115-119.	1.9	115
75	Effects of magnetism and doping on the electron-phonon coupling in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BaFe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2010, 82, .	3.2	112
76	NMR Chemical Shifts of Ice and Liquid Water:Â The Effects of Condensation. Journal of the American Chemical Society, 2000, 122, 123-129.	13.7	109
77	Adiabatic and nonadiabatic phonon dispersion in a Wannier function approach. Physical Review B, 2010, 82, .	3.2	108
78	Phonon-limited resistivity of graphene by first-principles calculations: Electron-phonon interactions, strain-induced gauge field, and Boltzmann equation. Physical Review B, 2014, 90, .	3.2	105
79	Density-functional theory of the nonlinear optical susceptibility: Application to cubic semiconductors. Physical Review B, 1996, 53, 15638-15642.	3.2	103
80	First-Principles Calculation of the17O NMR Parameters in Ca Oxide and Ca Aluminosilicates:Â the Partially Covalent Nature of the Caâ^'O Bond, a Challenge for Density Functional Theory. Journal of the American Chemical Society, 2004, 126, 12628-12635.	13.7	103
81	Kohn anomalies and nonadiabaticity in doped carbon nanotubes. Physical Review B, 2007, 75, .	3.2	103
82	Second-order structural phase transitions, free energy curvature, and temperature-dependent anharmonic phonons in the self-consistent harmonic approximation: Theory and stochastic implementation. Physical Review B, 2017, 96, .	3.2	100
83	Position and momentum mapping of vibrations in graphene nanostructures. Nature, 2019, 573, 247-250.	27.8	96
84	Structure, Bonding, and Geochemistry of Xenon at High Pressures. Science, 1997, 277, 930-933.	12.6	94
85	Strong anharmonicity induces quantum melting of charge density wave in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>2</mml:mn><mml:mi>H</mml:mi><mml:mo>-</mml:mo></mml:mrow></mml:math> pressure. Physical Review B, 2015, 92, .	3.2	93
86	Evidence for Flat Bands near the Fermi Level in Epitaxial Rhombohedral Multilayer Graphene. ACS Nano, 2015, 9, 5432-5439.	14.6	92
87	Phonon Collapse and Second-Order Phase Transition in Thermoelectric SnSe. Physical Review Letters, 2019, 122, 075901.	7.8	92
88	Relativistic nuclear magnetic resonance chemical shifts of heavy nuclei with pseudopotentials and the zeroth-order regular approximation. Journal of Chemical Physics, 2003, 118, 5746-5753.	3.0	91
89	First-Principles Calculation of the 17O NMR Parameters of a Calcium Aluminosilicate Glass. Journal of Physical Chemistry B, 2005, 109, 6052-6060.	2.6	89
90	Anharmonic phonon frequency shift inMgB2. Physical Review B, 2003, 68, .	3.2	88

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91	Combinedab initio computational and experimental multinuclear solid-state magnetic resonance study of phenylphosphonic acid. Magnetic Resonance in Chemistry, 2004, 42, 445-452.	1.9	88
92	Density functional theory description of hole-trapping inSiO2: A self-interaction-corrected approach. Physical Review B, 2005, 71, .	3.2	86
93	First-principles calculation of lattice thermal conductivity in crystalline phase change materials: GeTe, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="bold">Sb</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">Te</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> , and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mat	3.2	86
94	Structure and stability of graphene nanoribbons in oxygen, carbon dioxide, water, and ammonia. Physical Review B, 2010, 82, .	3.2	85
95	Superconductivity from doping boron icosahedra. Physical Review B, 2004, 69, .	3.2	84
96	Doped Graphene as Tunable Electronâ^'Phonon Coupling Material. Nano Letters, 2010, 10, 1172-1176.	9.1	84
97	Theoretical Investigation of Oxygen-17 NMR Shielding and Electric Field Gradients in Glutamic Acid Polymorphs. Journal of Physical Chemistry A, 2004, 108, 6032-6037.	2.5	83
98	First-principles study of OH-stretching modes in kaolinite, dickite, and nacrite. American Mineralogist, 2005, 90, 50-60.	1.9	83
99	New perspectives on calcium environments in inorganic materials containing calciumâ€“oxygen bonds: A combined computationalâ€“experimental 43Ca NMR approach. Chemical Physics Letters, 2008, 464, 42-48.	2.6	83
100	Phonon surface mapping of graphite: Disentangling quasi-degenerate phonon dispersions. Physical Review B, 2009, 80, .	3.2	83
101	Complete 1H resonance assignment of Î²-maltose from 1Hâ€“1H DQ-SQ CRAMPS and 1H (DQ-DUMBO)â€“13C SQ refocused INEPT 2D solid-state NMR spectra and first principles GIPAW calculations. Physical Chemistry Chemical Physics, 2010, 12, 6970.	2.8	83
102	Magnetic Susceptibility of Insulators from First Principles. Physical Review Letters, 1996, 76, 4246-4249.	7.8	82
103	Calcium Phosphates and Hydroxyapatite: Solid-State NMR Experiments and First-Principles Calculations. Applied Magnetic Resonance, 2007, 32, 435-457.	1.2	82
104	High-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>T</mml:mi><mml:mi>c</mml:mi></mml:msub></mml:math>Superconductivity in Superhard Diamondlike<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BC</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2008, 101, 016401.	7.8	81
105	Intercalant and Intermolecular Phonon Assisted Superconductivity in K-Doped Picene. Physical Review Letters, 2011, 107, 137006.	7.8	79
106	Current-voltage characteristics of graphene devices: Interplay between Zener-Klein tunneling and defects. Physical Review B, 2010, 82, .	3.2	78
107	First-principles theory of orbital magnetization. Physical Review B, 2010, 81, .	3.2	77
108	A first principles theory of nuclear magnetic resonance J-coupling in solid-state systems. Journal of Chemical Physics, 2007, 127, 204107.	3.0	76

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109	First-Principles Nuclear Magnetic Resonance Structural Analysis of Vitreous Silica. Journal of Physical Chemistry C, 2009, 113, 7917-7929.	3.1	76
110	Giant Nonadiabatic Effects in Layer Metals: Raman Spectra of Intercalated Graphite Explained. Physical Review Letters, 2008, 100, 226401.	7.8	75
111	Anharmonic effects in atomic hydrogen: Superconductivity and lattice dynamical stability. Physical Review B, 2016, 93, .	3.2	75
112	Large Scale Quantum Simulations:C60Impacts on a Semiconducting Surface. Physical Review Letters, 1994, 73, 3471-3474.	7.8	72
113	Intrinsic charge transfer gap in NiO from<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mtext>Ni</mml:mtext><mml:mtext>â€‰</mml:mtext><mml:mi>K</mml:mi></mml:math>-edge x-ray absorption spectroscopy. Physical Review B, 2009, 79, .	3.2	72
114	Raman spectroscopy of graphene under ultrafast laser excitation. Nature Communications, 2018, 9, 308.	12.8	70
115	The stochastic self-consistent harmonic approximation: calculating vibrational properties of materials with full quantum and anharmonic effects. Journal of Physics Condensed Matter, 2021, 33, 363001.	1.8	70
116	Structural and electronic relaxations around substitutionalCr3+andFe3+ions in corundum. Physical Review B, 2003, 67, .	3.2	69
117	Magnetic response and NMR spectra of carbon nanotubes fromab initiocalculations. Physical Review B, 2006, 73, .	3.2	69
118	Investigation of the Interface in Silica-Encapsulated Liposomes by Combining Solid State NMR and First Principles Calculations. Journal of the American Chemical Society, 2011, 133, 16815-16827.	13.7	69
119	First-Principles Study of Excitonic Self-Trapping in Diamond. Physical Review Letters, 1995, 75, 3166-3169.	7.8	67
120	Phonon Softening and Superconductivity in Tellurium under Pressure. Physical Review Letters, 1996, 77, 1151-1154.	7.8	67
121	First-principles calculation of the infrared spectrum of lizardite. American Mineralogist, 2002, 87, 1286-1290.	1.9	66
122	First-principles calculations of phonon frequencies, lifetimes, and spectral functions from weak to strong anharmonicity: The example of palladium hydrides. Physical Review B, 2015, 91, .	3.2	66
123	Ab initioNMR Chemical Shift of Diamond, Chemical-Vapor-Deposited Diamond, and Amorphous Carbon. Physical Review Letters, 1997, 79, 2340-2343.	7.8	65
124	NMR Chemical Shifts in Hard Carbon Nitride Compounds. Physical Review Letters, 1998, 80, 3388-3391.	7.8	65
125	Strong anharmonicity in the phonon spectra of PbTe and SnTe from first principles. Physical Review B, 2018, 97, .	3.2	63
126	First-Principles Calculation of17O and25Mg NMR Shieldings in MgO at Finite Temperature: Rovibrational Effect in Solids. Journal of Physical Chemistry B, 2005, 109, 7245-7250.	2.6	62

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127	Quantum Enhancement of Charge Density Wave in NbS₂ in the Two-Dimensional Limit. Nano Letters, 2019, 19, 3098-3103.	9.1	62
128	The effect of radiation damage on local structure in the crystalline fraction of ZrSiO₄: Investigating the²⁹Si NMR response to pressure in zircon and reidite. American Mineralogist, 2003, 88, 1663-1667.	1.9	61
129	First-principles calculation of the infrared spectrum of hematite. American Mineralogist, 2008, 93, 1019-1027.	1.9	61
130	Hidden polymorphs drive vitrification in B2O3. Nature Materials, 2012, 11, 925-929.	27.5	60
131	Signature of the two-dimensional phonon dispersion in graphene probed by double-resonant Raman scattering. Physical Review B, 2013, 87, .	3.2	60
132	Ab Initio Calculations of NMR Parameters of Highly Coordinated Oxygen Sites in Aluminosilicates. Journal of Physical Chemistry B, 2004, 108, 13249-13253.	2.6	57
133	Possibility of superconductivity in graphite intercalated with alkaline earths investigated with density functional theory. Physical Review B, 2006, 74, .	3.2	57
134	Electronic structure of heavily doped graphene: The role of foreign atom states. Physical Review B, 2007, 76, .	3.2	57
135	Structural properties of lithium and sodium tetrasilicate glasses: Molecular dynamics simulations versus NMR experimental and first-principles data. Solid State Sciences, 2010, 12, 183-192.	3.2	56
136	Electronic and vibrational properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TiSe</mml:mi><mml:mn>2</mml:mn></mml:msub></mm the charge-density-wave phase from first principles. Physical Review B, 2015, 92, .	3.2	56
137	Pressure and stress tensor of complex anharmonic crystals within the stochastic self-consistent harmonic approximation. Physical Review B, 2018, 98, .	3.2	56
138	First-principles calculation of H/D isotopic fractionation between hydrous minerals and water. Geochimica Et Cosmochimica Acta, 2010, 74, 3874-3882.	3.9	55
139	Equilibrium magnesium isotope fractionation between aqueous Mg2+ and carbonate minerals: Insights from path integral molecular dynamics. Geochimica Et Cosmochimica Acta, 2015, 163, 126-139.	3.9	55
140	Critical Role of the Exchange Interaction for the Electronic Structure and Charge-Density-Wave Formation in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>TiSe</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></m Physical Review Letters, 2017, 119, 176401.	7.8	55
141	Magnetic susceptibility of semiconductors by an all-electron first-principles approach. Physical Review B, 1997, 56, 1009-1012.	3.2	54
142	Theoretical infrared absorption coefficient of OH groups in minerals. American Mineralogist, 2008, 93, 950-953.	1.9	54
143	Implementation of High Resolution ⁴³Ca Solid State NMR Spectroscopy: Toward the Elucidation of Calcium Sites in Biological Materials. Journal of the American Chemical Society, 2009, 131, 13430-13440.	13.7	54
144	Nonlocal Pseudopotentials and Magnetic Fields. Physical Review Letters, 2003, 91, 196401.	7.8	53

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145	Electron-phonon coupling and phonon self-energy inMgB2: Interpretation ofMgB2Raman spectra. Physical Review B, 2005, 71, .	3.2	53
146	Laser without population inversion and coherent trapping. Optics Communications, 1991, 84, 393-400.	2.1	51
147	Spin and orbital magnetic response in metals: Susceptibility and NMR shifts. Physical Review B, 2007, 76, .	3.2	51
148	Ab initio resonant Raman spectra of diamond-like carbons. Diamond and Related Materials, 2005, 14, 1078-1083.	3.9	49
149	A biocompatible calcium bisphosphonate coordination polymer: towards a metal-linker synergistic therapeutic effect?. CrystEngComm, 2013, 15, 9899.	2.6	49
150	Magnetic gap opening in rhombohedral-stacked multilayer graphene from first principles. Physical Review B, 2017, 95, .	3.2	48
151	Anharmonic and non-adiabatic effects in MgB2: Implications for the isotope effect and interpretation of Raman spectra. Physica C: Superconductivity and Its Applications, 2007, 456, 38-44.	1.2	47
152	Structural relaxations around Ti, Cr and Fe impurities in Î±-Al2O3probed by x-ray absorption near-edge structure combined with first-principles calculations. Journal of Physics Condensed Matter, 2005, 17, 5467-5480.	1.8	46
153	Electrochemical doping of few-layer ZrNCl from first principles: Electronic and structural properties in field-effect configuration. Physical Review B, 2014, 89, .	3.2	46
154	Flat electronic bands in long sequences of rhombohedral-stacked graphene. Physical Review B, 2018, 97, .	3.2	46
155	OxygenK-edge XANES of germanates investigated using first-principles calculations. Physical Review B, 2007, 75, .	3.2	43
156	First principles NMR calculations of phenylphosphinic acid C6H5HPO(OH): Assignments, orientation of tensors by local field experiments and effect of molecular motion. Journal of Magnetic Resonance, 2007, 187, 131-140.	2.1	43
157	Optomechanical Measurement of Thermal Transport in Two-Dimensional MoSe₂ Lattices. Nano Letters, 2019, 19, 3143-3150.	9.1	43
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