Matteo Calandra

List of Publications by Year
in descending order

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139 papers	31,419 citations	28274 55 h-index	10734 138 g-index
141 all docs	141 docs citations	141 times ranked	27028 citing authors

#	Article	IF	Citations
1	Gate-Tunable Magnetism and Giant Magnetoresistance in Suspended Rhombohedral-Stacked Few-Layer Graphene. Nano Letters, 2022, 22, 5094-5099.	9.1	12
2	Theory of ultrafast magnetization of nonmagnetic semiconductors with localized conduction bands. Physical Review B, 2022, 105, .	3.2	1
3	Misfit Layer Compounds: A Platform for Heavily Doped 2D Transition Metal Dichalcogenides. Advanced Functional Materials, 2021, 31, 2007706.	14.9	17
4	Black metal hydrogen above 360â€‰GPa driven by proton quantum fluctuations. Nature Physics, 2021, 17, 63-67.	16.7	40
5	Electronic structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">TiSe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> from a quasi-self-consistent <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:msub></mml:mrow></mml:math> approach. Physical Review B, 2021, 103, .	3.2	8
6	Ab-initio energetics of graphite and multilayer graphene: stability of Bernal versus rhombohedral stacking. 2D Materials, 2021, 8, 035006.	4.4	7
7	Anomalous Highâ€Temperature Superconductivity in YH₆. Advanced Materials, 2021, 33, e2006832.	21.0	196
8	2D Monolayer of the 1Tâ€™ Phase of Alloyed WSSe from Colloidal Synthesis. Journal of Physical Chemistry C, 2021, 125, 11058-11065.	3.1	9
9	Intrinsic Vibrational Angular Momentum from Nonadiabatic Effects in Noncollinear Magnetic Molecules. Physical Review Letters, 2021, 126, 225703.	7.8	10
10	Charge density wave in single-layer Pb/Ge(111) driven by Pb-substrate exchange interaction. Physical Review B, 2021, 104, .	3.2	3
11	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
12	van der Waals driven anharmonic melting of the 3D charge density wave in VSe2. Nature Communications, 2021, 12, 598.	12.8	28
13	Lattice dynamics of photoexcited insulators from constrained density-functional perturbation theory. Physical Review B, 2021, 104, .	3.2	8
14	Dominant Role of Quantum Anharmonicity in the Stability and Optical Properties of Infinite Linear Acetylenic Carbon Chains. Journal of Physical Chemistry Letters, 2021, 12, 10339-10345.	4.6	10
15	Polar magnetic metallic state in few-layer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BiFeO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> Physical Review B, 2021, 104, .	3.2	4
16	Light-Tunable Charge Density Wave Orders in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>MoTe</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>WTe</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow> Weak Dimensionality Dependence and Dominant Role of Ionic Fluctuations in the Charge-Density-Wave Transition of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>NbSe</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow> Physical Review Letters, 2020, 125, 106101.	7.8	37
17	Thermal conductivity of Bi2Se3 from bulk to thin films: Theory and experiment. Physical Review B, 2020, 101, .	3.2	10
18			

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19	Long-Range Rhombohedral-Stacked Graphene through Shear. Nano Letters, 2020, 20, 5017-5023.	9.1	12
20	Anharmonicity and Doping Melt the Charge Density Wave in Single-Layer TiSe₂. Nano Letters, 2020, 20, 4809-4815.	9.1	24
21	Hybrid-functional electronic structure of multilayer graphene. Physical Review B, 2020, 101, .	3.2	7
22	Quantum crystal structure in the 250-kelvin superconducting lanthanum hydride. Nature, 2020, 578, 66-69.	27.8	193
23	Theory of the thickness dependence of the charge density wave transition in 1 T-TiTe₂. 2D Materials, 2020, 7, 045032.	4.4	17
24	Electronic structure of pristine and Ni-substituted <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>La</mml:mi><mml:mi>Fe</mml:mi><mml:msub><mml:m mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> from near edge x-ray absorption fine structure experiments and first-principles simulations. Physical Review Research, 2020, 2, .	3.6	17
25	Electronic structure and magnetic properties of few-layer Cr ₂ Ge ₂ Te ₆ : the key role of nonlocal electronâ€“electron interaction effects. 2D Materials, 2019, 6, 045042.	4.4	36
26	Electric field exfoliation and high-TC superconductivity in field-effect hole-doped hydrogenated diamond (111). Applied Surface Science, 2019, 496, 143709.	6.1	8
27	Ab initio study of the LiH phase diagram at extreme pressures and temperatures. Physical Review B, 2019, 99, .	3.2	5
28	Charge density wave and spin 1/2 insulating state in single layer 1T-NbS ₂. 2D Materials, 2019, 6, 035041.	4.4	27
29	Quantum Enhancement of Charge Density Wave in NbS₂ in the Two-Dimensional Limit. Nano Letters, 2019, 19, 3098-3103.	9.1	62
30	Phonon Collapse and Second-Order Phase Transition in Thermoelectric SnSe. Physical Review Letters, 2019, 122, 075901.	7.8	92
31	Strong anharmonicity and high thermoelectric efficiency in high-temperature SnS from first principles. Physical Review B, 2019, 100, .	3.2	35
32	Quantum effects in muon spin spectroscopy within the stochastic self-consistent harmonic approximation. Physical Review Materials, 2019, 3, .	2.4	13
33	Electronic band structure of Two-Dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">WS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> /Graphene van der Waals Heterostructures. Physical Review B, 2018, 97, .	3.2	63
34	Energy relaxation mechanism of hot-electron ensembles in GaAs: Theoretical and experimental study of its temperature dependence. Physical Review B, 2018, 97, .	3.2	16
35	Strong anharmonicity in the phonon spectra of PbTe and SnTe from first principles. Physical Review B, 2018, 97, .	3.2	63
36	Exchange Enhancement of the Electronâ€“Phonon Interaction: The Case of Weakly Doped Two-Dimensional Multivalley Semiconductors. Journal of the Physical Society of Japan, 2018, 87, 041013.	1.6	0

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37	Multi-scale theoretical approach to X-ray absorption spectra in disordered systems: an application to the study of Zn(ii) in water. Physical Chemistry Chemical Physics, 2018, 20, 24775-24782.	2.8	10
38	Flat electronic bands in long sequences of rhombohedral-stacked graphene. Physical Review B, 2018, 97, .	3.2	46
39	Pressure and stress tensor of complex anharmonic crystals within the stochastic self-consistent harmonic approximation. Physical Review B, 2018, 98, .	3.2	56
40	Phonon-Assisted Magnetic Mott-Insulating State in the Charge Density Wave Phase of Single-Layer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>1</mml:mn><mml:mi>T</mml:mi><mml:mtext>â^'</mml:mtext><mml:msub><mml:mrow><m Physical Review Letters, 2018, 121, 026401.	7.8	52
41	Superconductivity and Charge Density Wave Phase of the Correlated Metallic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Pb</mml:mi><mml:mrow><mml:mo>/</mml:mo><mml:mi>Si</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mn>111</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 572 Td (stretchy="fals Letters, 2018, 120, 196402.	7.8	15
42	Field-effect-driven half-metallic multilayer graphene. Physical Review B, 2018, 98, .	3.2	10
43	High-pressure phase diagram of hydrogen and deuterium sulfides from first principles: Structural and vibrational properties including quantum and anharmonic effects. Physical Review B, 2018, 97, .	3.2	38
44	Magnetic gap opening in rhombohedral-stacked multilayer graphene from first principles. Physical Review B, 2017, 95, .	3.2	48
45	Breakdown of Optical Phononsâ€™ Splitting in Two-Dimensional Materials. Nano Letters, 2017, 17, 3758-3763.	9.1	127
46	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	1.8	4,303
47	X-ray magnetic and natural circular dichroism from first principles: Calculation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>K</mml:mi></mml:math> - and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>L</mml:mi><mml:mn>1</mml:mn></mml:msub></mml -edge spectra. Physical Review B, 2017, 96, .	3.2	18
48	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
49	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
50	Effect of electron doping on lattice instabilities in single-layer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>H</mml:mi><mml:mo Physical Review B, 2017, 95, .	3.2	86
51	High- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>T</mml:mi><mml:mi>c</mml:mi></mml:msub superconductivity in weakly electron-doped HfNCl. Physical Review B, 2017, 96, .	3.2	5
52	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></ Physical Review Letters, 2017, 119, 176401.	7.8	55
53	Anharmonicity and the isotope effect in superconducting lithium at high pressures: A first-principles approach. Physical Review B, 2017, 96, .	3.2	4
54	Inelastic X ray scattering under pressure to probe the quantum phase transition in the transition metal dichalcogenides. Journal of Physics: Conference Series, 2017, 950, 032017.	0.4	0

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55	First-principles determination of the Raman fingerprint of rhombohedral graphite. Physical Review Materials, 2017, 1, .	2.4	19
56	Anharmonic enhancement of superconductivity in metallic molecularCmcaâ€‰â€‰âˆ’â€‰â€‰4 hydrogen at high pressure: a first-principles study. Journal of Physics Condensed Matter, 2016, 28, 494001.	1.8	26
57	Two-dimensional FrÃ¶hlich interaction in transition-metal dichalcogenide monolayers: Theoretical modeling and first-principles calculations. Physical Review B, 2016, 94, .	3.2	155
58	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
59	Determination of scattering time and of valley occupation in transition-metal dichalcogenides doped by field effect. Physical Review B, 2016, 93, .	3.2	9
60	Formation of hot-electron ensembles quasiequilibrated in momentum space by ultrafast momentum scattering of highly excited hot electrons photoinjected into the Î“ valley of GaAs. Physical Review B, 2016, 93, .	3.2	37
61	Anharmonic effects in atomic hydrogen: Superconductivity and lattice dynamical stability. Physical Review B, 2016, 93, .	3.2	75
62	Spin susceptibility and electron-phonon coupling of two-dimensional materials by range-separated hybrid density functionals: Case study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>Li</mml:mi></mml:mrow><mml:mi>x</mml: Physical Review B, 2016, 94, .	3.2	5
63	Atomic and electronic structure of trilayer graphene/SiC(0001): Evidence of Strong Dependence on Stacking Sequence and charge transfer. Scientific Reports, 2016, 6, 33487.	3.3	16
64	Quantum hydrogen-bond symmetrization in the superconducting hydrogen sulfide system. Nature, 2016, 532, 81-84.	27.8	222
65	Wannier interpolation of the electron-phonon matrix elements in polar semiconductors: Polar-optical coupling in GaAs. Physical Review B, 2015, 92, .	3.2	126
66	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
67	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>â€'</mml: pressure. Physical Review B, 2015, 92, .	3.2	93
68	Density-functional calculation of static screening in two-dimensional materials: The long-wavelength dielectric function of graphene. Physical Review B, 2015, 91, .	3.2	21
69	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
70	Universal Increase in the Superconducting Critical Temperature of Two-Dimensional Semiconductors at Low Doping by the Electron-Electron Interaction. Physical Review Letters, 2015, 114, 077001.	7.8	14
71	Charge density waves go nano. Nature Nanotechnology, 2015, 10, 737-738.	31.5	16
72	Evidence for Flat Bands near the Fermi Level in Epitaxial Rhombohedral Multilayer Graphene. ACS Nano, 2015, 9, 5432-5439.	14.6	92

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73	High-Pressure Hydrogen Sulfide from First Principles: A Strongly Anharmonic Phonon-Mediated Superconductor. Physical Review Letters, 2015, 114, 157004.	7.8	377
74	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
75	Calandra and Mauri Reply. Physical Review Letters, 2014, 112, 049702.	7.8	4
76	Huge anharmonic effects in superconducting hydrides and transition metal dichalcogenides. Physica Status Solidi (B): Basic Research, 2014, 251, 2556-2562.	1.5	2
77	Two-Dimensional Analysis of the Double-Resonant 2D Raman Mode in Bilayer Graphene. Physical Review Letters, 2014, 113, 187401.	7.8	35
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	Possible phase separation and weak localization in the absence of a charge-density wave in single-phase<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>T</mml:mi></mml:mrow> xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>VS</mml:mi><mml:mn>2</mml:mn></mml:msub> Physical Review B, 2014, 89, .	3.2	28
80	Electronâ€“Phonon Interactions and the Intrinsic Electrical Resistivity of Graphene. Nano Letters, 2014, 14, 1113-1119.	9.1	149
81	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
82	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
83	First-Principles Theory of Anharmonicity and the Inverse Isotope Effect in Superconducting Palladium-Hydride Compounds. Physical Review Letters, 2013, 111, 177002.	7.8	173
84	Chemically exfoliated single-layer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mtext>MoS</mml:mtext> Stability, lattice dynamics, and catalytic adsorption from first principles. Physical Review B, 2013, 88, .	3.2	240
85	Anharmonic phonons in few-layer MoS<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>: Raman spectroscopy of ultralow energy compression and shear modes. Physical Review B, 2013, 87, .	3.2	90
86	Projector augmented wave calculation of x-ray absorption spectra at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>L</mml:mi><mml:mrow><mml:mn>2</mml:mn><mml:mo>,</mml:mo><mml:mn>3</mml:mn> Physical Review B, 2013, 87, .	3.2	59
87	display="inline"><mml:msub><mml:mrow /><mml:mn>14</mml:mn></mml:msub></mml:math>Cu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>24</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow	3.2	7
88	Comment on â€œElectronic Structure of SuperconductingKC8and NonsuperconductingLiC6Graphite Intercalation Compounds: Evidence for a Graphene-Sheet-Driven Superconducting Stateâ€• Physical Review Letters, 2012, 108, 149701; discussion 149702.	7.8	7
89	Local and nonlocal electron-phonon couplings in K<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>picene and the effect of metallic screening. Physical Review B, 2012, 86, .	3.2	25
90	Anharmonic suppression of charge density waves in 2<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>H</mml:mi></mml:mrow></mml:math>-NbS<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>. Physical Review B, 2012, 86, .	3.2	66

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91	Superconductivity in metalâ€coated graphene. Physica Status Solidi (B): Basic Research, 2012, 249, 2544-2548.	1.5	12
92	Understanding the Photomagnetic Behavior in Copper Octacyanomolybdates. Journal of Physical Chemistry A, 2012, 116, 8678-8683.	2.5	23
93	Phonon-mediated superconductivity in graphene by lithium deposition. Nature Physics, 2012, 8, 131-134.	16.7	431
94	K-edge x-ray absorption spectra in transition-metal oxides beyond the single-particle approximation: Shake-up many-body effects. Physical Review B, 2012, 86, .	3.2	30
95	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
96	Intercalant and Intermolecular Phonon Assisted Superconductivity in K-Doped Picene. Physical Review Letters, 2011, 107, 137006.	7.8	79
97	Comparative study of the phonons in nonsuperconducting BaC<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>6</mml:mn></mml:msub></mml:math>and superconducting CaC<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>6</mml:mn></mml:msub></mml:math>using inelastic x-ray scattering. Physical Review B, 2011, 84, .	3.2	14
98	Angular dependence of core hole screening in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LiCoO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>: A<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>DFT</mml:mtext><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math>study of the oxygen and cobalt<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="i. Phy	3.2	90
99	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
100	Multiple pre-edge structures in Cu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>K</mml:mi></mml:math>-edge x-ray absorption spectra of 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>cuprate revealed by high-resolution x-ray absorption spectroscopy. Physical Review B, 2010, 81, .	3.2	2
101	Phonon dispersion and low-energy anomaly in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CaC</mml:mtext></mml:mrow><mml:mn>6</mml:mn></mml:msub></mml:mrow></mml:math>: inelastic neutron and x-ray scattering experiments. Physical Review B, 2010, 81, .	3.2	12
102	Neutron scattering study of the high-energy graphitic phonons in superconducting<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CaC</mml:mtext></mml:mrow><mml:mn>6</mml:mn></mml:msub></mml:mrow></mml:math>: Physical Review B, 2010, 82, .	3.2	14
103	High Pressure and Superconductivity: Intercalated Graphite Cac6 as a Model System. NATO Science for Peace and Security Series B: Physics and Biophysics, 2010, , 407-418.	0.3	0
104	Adiabatic and nonadiabatic phonon dispersion in a Wannier function approach. Physical Review B, 2010, 82, .	3.2	108
105	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>	3.2	184
106	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>compou Physical Review B, 2009, 80, .	3.2	150
107	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
108	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

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109	Thermodynamic stabilities of ternary metal borides: Anab initioguide for synthesizing layered superconductors. Physical Review B, 2008, 78, .	3.2	29
110	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
111	Giant Nonadiabatic Effects in Layer Metals: Raman Spectra of Intercalated Graphite Explained. Physical Review Letters, 2008, 100, 226401.	7.8	75
112	Maximum<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>at the verge of a simultaneous order-disorder and lattice-softening transition in superconducting<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CaC</mml:mtext></mml:mrow><mml:mn>6</mml:mn></mml:msub></mml:mrow></mml:ms Physical Review B, 2008, 78, .	3.2	16
113	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
114	Exponential Localization of Wannier Functions in Insulators. Physical Review Letters, 2007, 98, 046402.	7.8	297
115	Publisher's Note: Electronic structure of heavily doped graphene: The role of foreign atom states [Phys. Rev. B76, 161406 (2007)]. Physical Review B, 2007, 76, .	3.2	7
116	Search for highTcin layered structures: The case of LiB. Physical Review B, 2007, 75, .	3.2	35
117	Weak anharmonic effects inMgB2: A comparative inelastic x-ray scattering and Raman study. Physical Review B, 2007, 75, .	3.2	41
118	Electronic structure of heavily doped graphene: The role of foreign atom states. Physical Review B, 2007, 76, .	3.2	57
119	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
120	Electronic thermal conductivity at high temperatures: Violation of the Wiedemann-Franz law in narrow-band metals. Physical Review B, 2006, 74, .	3.2	11
121	Possibility of superconductivity in graphite intercalated with alkaline earths investigated with density functional theory. Physical Review B, 2006, 74, .	3.2	57
122	Origin of superconductivity of CaC6 and of other intercalated graphites. Physica Status Solidi (B): Basic Research, 2006, 243, 3458-3463.	1.5	12
123	Polarized Resonant Inelastic X-Ray Scattering as an Ultrafine Probe of Excited States ofLa2CuO4. Physical Review Letters, 2006, 96, 077006.	7.8	34
124	Phonon softening inNaxCoO2âˆ™yH2O: Implications for the Fermi surface topology and the superconducting state. Physical Review B, 2006, 74, .	3.2	19
125	Density functional theory description of hole-trapping inSiO2: A self-interaction-corrected approach. Physical Review B, 2005, 71, .	3.2	86
126	Electron-phonon coupling and phonon self-energy inMgB2: Interpretation ofMgB2Raman spectra. Physical Review B, 2005, 71, .	3.2	53

#	Article	IF	Citations
127	Theoretical Explanation of Superconductivity inC6Ca. Physical Review Letters, 2005, 95, 237002.	7.8	223
128	Superconductivity from doping boron icosahedra. Physical Review B, 2004, 69, .	3.2	84
129	Phonon Dispersion and Lifetimes inMgB2. Physical Review Letters, 2003, 90, 095506.	7.8	139
130	Colloquium: Saturation of electrical resistivity. Reviews of Modern Physics, 2003, 75, 1085-1099.	45.6	369
131	Anharmonic phonon frequency shift inMgB2. Physical Review B, 2003, 68, .	3.2	88
132	Dynamical properties of a strongly correlated model for quarter-filled layered organic molecular crystals. Physical Review B, 2003, 68, .	3.2	46
133	Violation of Ioffe-Regel condition but saturation of resistivity of the high- T c cuprates. Europhysics Letters, 2003, 61, 88-94.	2.0	25
134	Metal-insulator transition and charge ordering in the extended Hubbard model at one-quarter filling. Physical Review B, 2002, 66, .	3.2	40
135	Electrical resistivity at large temperatures: Saturation and lack thereof. Physical Review B, 2002, 66, .	3.2	46
136	Saturation of Electrical Resistivity in Metals at Large Temperatures. Physical Review Letters, 2001, 87, 266601.	7.8	20
137	From antiferromagnetism tod-wave superconductivity in the two-dimensionalt-Jmodel. Physical Review B, 2000, 61, R11894-R11897.	3.2	30
138	Numerical study of the two-dimensional Heisenberg model using a Green function Monte Carlo technique with a fixed number of walkers. Physical Review B, 1998, 57, 11446-11456.	3.2	154
139	Charge Fluctuations Close to Phase Separation in the Two-Dimensionaltâ^'JModel. Physical Review Letters, 1998, 81, 5185-5188.	7.8	58