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	Excitonic-insulator instability and Peierls distortion in one-dimensional semimetals. Physical Review B, 2022, 105, .	3.2	2
2	Nonperturbative Green's function method to determine the electronic spectral function due to electron-phonon interactions: Application to a graphene model from weak to strong coupling. Physical Review B, 2022, 105, .	3.2	1
3	Gate-Tunable Magnetism and Giant Magnetoresistance in Suspended Rhombohedral-Stacked Few-Layer Graphene. Nano Letters, 2022, 22, 5094-5099.	9.1	12
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:mn></mml:mrow> 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	Time-dependent self-consistent harmonic approximation: Anharmonic nuclear quantum dynamics and time correlation functions. Physical Review B, 2021, 103, .	3.2	19
8	Anomalous Highâ€Temperature Superconductivity in YH₆. Advanced Materials, 2021, 33, e2006832.	21.0	196
9	First-principles theory of infrared vibrational spectroscopy of metals and semimetals: Application to graphite. Physical Review B, 2021, 103, .	3.2	9
10	Intrinsic Vibrational Angular Momentum from Nonadiabatic Effects in Noncollinear Magnetic Molecules. Physical Review Letters, 2021, 126, 225703.	7.8	10
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	The microscopic origin of the anomalous isotopic properties of ice relies on the strong quantum anharmonic regime of atomic vibration. Journal of Chemical Physics, 2021, 155, 184502.	3.0	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	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:mn></mml:mrow> Physical Review Letters, 2020, 125, 106101.	7.8	37
16	Long-Range Rhombohedral-Stacked Graphene through Shear. Nano Letters, 2020, 20, 5017-5023.	9.1	12
17	Anharmonicity and Doping Melt the Charge Density Wave in Single-Layer TiSe₂. Nano Letters, 2020, 20, 4809-4815.	9.1	24
18	Hybrid-functional electronic structure of multilayer graphene. Physical Review B, 2020, 101, .	3.2	7

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19	Quantum crystal structure in the 250-kelvin superconducting lanthanum hydride. Nature, 2020, 578, 66-69.	27.8	193
20	Theory of the thickness dependence of the charge density wave transition in 1 T-TiTe₂. 2D Materials, 2020, 7, 045032.	4.4	17
21	Position and momentum mapping of vibrations in graphene nanostructures. Nature, 2019, 573, 247-250.	27.8	96
22	Raman spectroscopy of graphene under ultrafast laser excitation. EPJ Web of Conferences, 2019, 205, 05003.	0.3	0
23	Giant effective charges and piezoelectricity in gapped graphene. 2D Materials, 2019, 6, 045015.	4.4	23
24	Nanoscale Vibrational Spectroscopy of Graphene by Large-q EELS. Microscopy and Microanalysis, 2019, 25, 612-613.	0.4	0
25	Electric field exfoliation and high-TC superconductivity in field-effect hole-doped hydrogenated diamond (111). Applied Surface Science, 2019, 496, 143709.	6.1	8
26	Ab initio study of the LiH phase diagram at extreme pressures and temperatures. Physical Review B, 2019, 99, .	3.2	5
27	Unified theory of thermal transport in crystals and glasses. Nature Physics, 2019, 15, 809-813.	16.7	255
28	Optomechanical Measurement of Thermal Transport in Two-Dimensional MoSe₂ Lattices. Nano Letters, 2019, 19, 3143-3150.	9.1	43
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	van der Waals forces stabilize low-energy polymorphism in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><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:mrow></mml:math> : Implications for the crystallization anomaly. Physical Review Materials, 2019, 3, .	2.4	9
33	Quantum effects in muon spin spectroscopy within the stochastic self-consistent harmonic approximation. Physical Review Materials, 2019, 3, .	2.4	13
34	Hydrodynamic Heat Transport Regime in Bismuth: A Theoretical Viewpoint. Physical Review Letters, 2018, 120, 075901.	7.8	21
35	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
36	Raman spectroscopy of graphene under ultrafast laser excitation. Nature Communications, 2018, 9, 308.	12.8	70

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37	Strong anharmonicity in the phonon spectra of PbTe and SnTe from first principles. Physical Review B, 2018, 97, .	3.2	63
38	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
39	Flat electronic bands in long sequences of rhombohedral-stacked graphene. Physical Review B, 2018, 97, .	3.2	46
40	Pressure and stress tensor of complex anharmonic crystals within the stochastic self-consistent harmonic approximation. Physical Review B, 2018, 98, .	3.2	56
41	Field-effect-driven half-metallic multilayer graphene. Physical Review B, 2018, 98, .	3.2	10
42	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
43	The double-resonance Raman spectra in single-chirality (n, m) carbon nanotubes. Carbon, 2017, 117, 41-45.	10.3	13
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	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
47	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	1.8	4,303
48	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:m -edge spectra. Physical Review B, 2017, 96, .	3.2	18
49	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
50	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
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></mml:m 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></mml:m 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	Phonon anomalies in Graphene induced by highly excited charge carriers. , 2017, , .		0

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55	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
56	First-principles determination of the Raman fingerprint of rhombohedral graphite. Physical Review Materials, 2017, 1, .	2.4	19
57	Predicting the thermal conductivity in a graphene nanoflake from its response to a thermal impulse. Physical Review B, 2016, 94, .	3.2	2
58	Anharmonic enhancement of superconductivity in metallic molecularCmcaâ€‰â€‰â^'â€‰â€‰4 hydrogen at high pressure: a first-principles study. Journal of Physics Condensed Matter, 2016, 28, 494001.	1.8	26
59	Two-dimensional FrÃ¶hlich interaction in transition-metal dichalcogenide monolayers: Theoretical modeling and first-principles calculations. Physical Review B, 2016, 94, .	3.2	155
60	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
61	Nanoscale mechanisms for the reduction of heat transport in bismuth. Physical Review B, 2016, 93, .	3.2	16
62	Determination of scattering time and of valley occupation in transition-metal dichalcogenides doped by field effect. Physical Review B, 2016, 93, .	3.2	9
63	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
64	Anharmonic effects in atomic hydrogen: Superconductivity and lattice dynamical stability. Physical Review B, 2016, 93, .	3.2	75
65	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:mi> Physical Review B, 2016, 94, .	3.2	5
66	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
67	Quantum hydrogen-bond symmetrization in the superconducting hydrogen sulfide system. Nature, 2016, 532, 81-84.	27.8	222
68	Wannier interpolation of the electron-phonon matrix elements in polar semiconductors: Polar-optical coupling in GaAs. Physical Review B, 2015, 92, .	3.2	126
69	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></ the charge-density-wave phase from first principles. Physical Review B, 2015, 92, .	3.2	56
70	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 pressure. Physical Review B, 2015, 92, .	3.2	98
71	Dispersion effects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SiO</mml:mi><mml:mn>2</mml:mn></mml:msub></ Anab initiostudy. Physical Review B, 2015, 92, .	3.2	27
72	Phonon effects on x-ray absorption and nuclear magnetic resonance spectroscopies. Physical Review B, 2015, 92, .	3.2	31

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73	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
74	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
75	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
76	Phonon hydrodynamics in two-dimensional materials. Nature Communications, 2015, 6, 6400.	12.8	385
77	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
78	Evidence for Flat Bands near the Fermi Level in Epitaxial Rhombohedral Multilayer Graphene. ACS Nano, 2015, 9, 5432-5439.	14.6	92
79	High-Pressure Hydrogen Sulfide from First Principles: A Strongly Anharmonic Phonon-Mediated Superconductor. Physical Review Letters, 2015, 114, 157004.	7.8	377
80	High-field transport in graphene: the impact of Zener tunneling. Journal of Physics Condensed Matter, 2015, 27, 164205.	1.8	16
81	Raman spectroscopy as probe of nanometre-scale strain variations in graphene. Nature Communications, 2015, 6, 8429.	12.8	341
82	Vertical and adiabatic excitations in anthracene from quantum Monte Carlo: Constrained energy minimization for structural and electronic excited-state properties in the JAGP ansatz. Journal of Chemical Physics, 2015, 142, 214109.	3.0	21
83	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
84	Downfolding electron-phonon Hamiltonians fromab initiocalculations: Application to<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">K</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>picene. Physical Review B, 2014, 90, .	3.2	14
85	Calandra and Mauri Reply. Physical Review Letters, 2014, 112, 049702.	7.8	4
86	Equilibrium fractionation of H and O isotopes in water from path integral molecular dynamics. Geochimica Et Cosmochimica Acta, 2014, 135, 203-216.	3.9	25
87	Huge anharmonic effects in superconducting hydrides and transition metal dichalcogenides. Physica Status Solidi (B): Basic Research, 2014, 251, 2556-2562.	1.5	2
88	Thermal Conductivity of Graphene and Graphite: Collective Excitations and Mean Free Paths. Nano Letters, 2014, 14, 6109-6114.	9.1	449
89	Two-Dimensional Analysis of the Double-Resonant 2D Raman Mode in Bilayer Graphene. Physical Review Letters, 2014, 113, 187401.	7.8	35
90	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

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91	Electronâ€“Phonon Interactions and the Intrinsic Electrical Resistivity of Graphene. Nano Letters, 2014, 14, 1113-1119.	9.1	149
92	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
93	Quantum Monte Carlo Study of the Protonated Water Dimer. Journal of Chemical Theory and Computation, 2014, 10, 1980-1993.	5.3	18
94	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
95	Ab initiovariational approach for evaluating lattice thermal conductivity. Physical Review B, 2013, 88, .	3.2	199
96	First-Principles Theory of Anharmonicity and the Inverse Isotope Effect in Superconducting Palladium-Hydride Compounds. Physical Review Letters, 2013, 111, 177002.	7.8	173
97	A biocompatible calcium bisphosphonate coordination polymer: towards a metal-linker synergistic therapeutic effect?. CrystEngComm, 2013, 15, 9899.	2.6	49
98	Signature of the two-dimensional phonon dispersion in graphene probed by double-resonant Raman scattering. Physical Review B, 2013, 87, .	3.2	60
99	Anharmonic properties from a generalized third-orderab initioapproach: Theory and applications to graphite and graphene. Physical Review B, 2013, 87, .	3.2	180
100	Structural study of calcium phosphonates: a combined synchrotron powder diffraction, solid-state NMR and first-principle calculations approach. CrystEngComm, 2013, 15, 8763.	2.6	26
101	Extended Czjzek model applied to NMR parameter distributions in sodium metaphosphate glass. Journal of Physics Condensed Matter, 2013, 25, 255402.	1.8	15
102	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
103	Zener tunneling in the electrical transport of quasimetallic carbon nanotubes. Physical Review B, 2012, 86, .	3.2	9
104	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
105	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
106	Superconductivity in metalâ€coated graphene. Physica Status Solidi (B): Basic Research, 2012, 249, 2544-2548.	1.5	12
107	Phonon-mediated superconductivity in graphene by lithium deposition. Nature Physics, 2012, 8, 131-134.	16.7	431
108	Hidden polymorphs drive vitrification in B2O3. Nature Materials, 2012, 11, 925-929.	27.5	60

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109	Comment on â€œNew data on equilibrium iron isotope fractionation among sulfides: Constraints on mechanisms of sulfide formation in hydrothermal and igneous systemsâ€• by V.B. Polyakov and D.M. Soultanov. Geochimica Et Cosmochimica Acta, 2012, 87, 356-359.	3.9	21
110	Characterizing intrinsic charges in top gated bilayer graphene device by Raman spectroscopy. Carbon, 2012, 50, 3435-3439.	10.3	22
111	High-resolution solid state NMR experiments for the characterization of calcium phosphate biomaterials and biominerals. Journal of Materials Research, 2011, 26, 2355-2368.	2.6	21
112	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
113	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
114	Structural properties of carbon nanotubes derived from<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mrow /><mml:mn>13</mml:mn></mml:msup></mml:math>C NMR. Physical Review B, 2011, 84, .	3.2	28
115	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
116	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
117	Magnesium incorporation into hydroxyapatite. Biomaterials, 2011, 32, 1826-1837.	11.4	296
118	Intercalant and Intermolecular Phonon Assisted Superconductivity in K-Doped Picene. Physical Review Letters, 2011, 107, 137006.	7.8	79
119	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
120	Structure and stability of graphene nanoribbons in oxygen, carbon dioxide, water, and ammonia. Physical Review B, 2010, 82, .	3.2	85
121	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>As<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, 2010, 82, .	3.2	112
122	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
123	New perspectives in the PAW/GIPAW approach: JP-O-Si coupling constants, antisymmetric parts of shift tensors and NQR predictions. Magnetic Resonance in Chemistry, 2010, 48, S86-S102.	1.9	42
124	First-principles calculations of NMR parameters for phosphate materials. Magnetic Resonance in Chemistry, 2010, 48, S142-S150.	1.9	28
125	Ab initiog-tensor calculation for paramagnetic surface states: hydrogen adsorption at Si surfaces. Physica Status Solidi C: Current Topics in Solid State Physics, 2010, 7, 157-160.	0.8	24
126	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Si</mml:mtext></mml:mrow><mml:mtext>C</mml:mtext></mml:msub></mml:mrow></mml:math>pairs in SiC identified as paramagnetic defects with strongly anisotropic orbital quenching. Physical Review B, 2010, 81, .	3.2	15

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127	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
128	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
129	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
130	Current-voltage characteristics of graphene devices: Interplay between Zener-Klein tunneling and defects. Physical Review B, 2010, 82, .	3.2	78
131	First-principles theory of orbital magnetization. Physical Review B, 2010, 81, .	3.2	77
132	First-principles calculation of H/D isotopic fractionation between hydrous minerals and water. Geochimica Et Cosmochimica Acta, 2010, 74, 3874-3882.	3.9	55
133	Clarâ€™s Theory, Ï€-Electron Distribution, and Geometry of Graphene Nanoribbons. Journal of the American Chemical Society, 2010, 132, 3440-3451.	13.7	219
134	Doped Graphene as Tunable Electronâ^'Phonon Coupling Material. Nano Letters, 2010, 10, 1172-1176.	9.1	84
135	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
136	Adiabatic and nonadiabatic phonon dispersion in a Wannier function approach. Physical Review B, 2010, 82, .	3.2	108
137	New insights into oxygen environments generated during phosphate glass alteration: a combined 17O MAS and MQMAS NMR and first principles calculations study. Physical Chemistry Chemical Physics, 2010, 12, 9053.	2.8	19
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