

# Matteo Calandra

## List of Publications by Year in descending order

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papers

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all docs

141  
docs citations

141  
times ranked

27028  
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	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	0.7	4,303
3	Phonon-mediated superconductivity in graphene by lithium deposition. Nature Physics, 2012, 8, 131-134.	6.5	431
4	High-Pressure Hydrogen Sulfide from First Principles: A Strongly Anharmonic Phonon-Mediated Superconductor. Physical Review Letters, 2015, 114, 157004.	2.9	377
5	Colloquium: Saturation of electrical resistivity. Reviews of Modern Physics, 2003, 75, 1085-1099.	16.4	369
6	Exponential Localization of Wannier Functions in Insulators. Physical Review Letters, 2007, 98, 046402.	2.9	297
7	Anharmonic free energies and phonon dispersions from the stochastic self-consistent harmonic approximation: Application to platinum and palladium hydrides. Physical Review B, 2014, 89, .	1.1	264
8	Chemically exfoliated single-layer $\text{MoS}_2$ stability, lattice dynamics, and catalytic adsorption from first principles. Physical Review B, 2013, 88, .	1.1	240
9	Theoretical Explanation of Superconductivity in $\text{C}_6\text{Ca}$ . Physical Review Letters, 2005, 95, 237002.	2.9	223
10	Quantum hydrogen-bond symmetrization in the superconducting hydrogen sulfide system. Nature, 2016, 532, 81-84.	18.7	222
11	Density functional perturbation theory for gated two-dimensional heterostructures: Theoretical developments and application to flexural phonons in graphene. Physical Review B, 2017, 96, .	1.1	198
12	Anomalous High-Temperature Superconductivity in $\text{YH}_6$ . Advanced Materials, 2021, 33, e2006832.	11.1	196
13	Quantum crystal structure in the 250-kelvin superconducting lanthanum hydride. Nature, 2020, 578, 66-69.	18.7	193
14	Electron-phonon coupling and electron self-energy in electron-doped graphene: Calculation of angular-resolved photoemission spectra. Physical Review B, 2007, 76, .	1.1	188
15	Effect of dimensionality on the charge-density wave in few-layer $\text{NbSe}_2$ . Physical Review B, 2009, 80, .	1.1	184
16	First-Principles Theory of Anharmonicity and the Inverse Isotope Effect in Superconducting Palladium-Hydride Compounds. Physical Review Letters, 2013, 111, 177002.	2.9	173
17	Charge-Density Wave and Superconducting Dome in $\text{TiSe}_2$ from Electron-Phonon Interaction. Physical Review Letters, 2011, 106, 196406.	2.9	159
18	Two-dimensional Fröhlich interaction in transition-metal dichalcogenide monolayers: Theoretical modeling and first-principles calculations. Physical Review B, 2016, 94, .	1.1	155

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19	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.	1.1	154
20	First-principles calculations of x-ray absorption in a scheme based on ultrasoft pseudopotentials: From $\hat{I}_{\pm}$ -quartz to high- $T_c$ superconductors. Physical Review B, 2009, 80, .	1.1	150
21	Electron-Phonon Interactions and the Intrinsic Electrical Resistivity of Graphene. Nano Letters, 2014, 14, 1113-1119.	4.5	149
22	Phonon Dispersion and Lifetimes in MgB <sub>2</sub> . Physical Review Letters, 2003, 90, 095506.	2.9	139
23	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, .	1.1	127
24	Breakdown of Optical Phonons' Splitting in Two-Dimensional Materials. Nano Letters, 2017, 17, 3758-3763.	4.5	127
25	Wannier interpolation of the electron-phonon matrix elements in polar semiconductors: Polar-optical coupling in GaAs. Physical Review B, 2015, 92, .	1.1	126
26	Dissociation products and structures of solid $H_2S$ at strong compression. Physical Review B, 2016, 93, .	1.1	119
27	Effects of magnetism and doping on the electron-phonon coupling in $BaFe_2As_2$ . Physical Review B, 2010, 82, .	1.1	112
28	Adiabatic and nonadiabatic phonon dispersion in a Wannier function approach. Physical Review B, 2010, 82, .	1.1	108
29	Phonon-limited resistivity of graphene by first-principles calculations: Electron-phonon interactions, strain-induced gauge field, and Boltzmann equation. Physical Review B, 2014, 90, .	1.1	105
30	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, .	1.1	100
31	Strong anharmonicity induces quantum melting of charge density wave in $HgTe$ under pressure. Physical Review B, 2015, 92, .		
32	Evidence for Flat Bands near the Fermi Level in Epitaxial Rhombohedral Multilayer Graphene. ACS Nano, 2015, 9, 5432-5439.	7.3	92
33	Phonon Collapse and Second-Order Phase Transition in Thermoelectric SnSe. Physical Review Letters, 2019, 122, 075901.	2.9	92
34	Angular dependence of core hole screening in $LiCoO_2$ . Physical Review B, 2013, 87, .	1.1	90
35	Anharmonic phonons in few-layer MoS <sub>2</sub> : Raman spectroscopy of ultralow energy compression and shear modes. Physical Review B, 2013, 87, .	1.1	90
36	Anharmonic phonon frequency shift in MgB <sub>2</sub> . Physical Review B, 2003, 68, .	1.1	88

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37	Density functional theory description of hole-trapping in SiO <sub>2</sub> : A self-interaction-corrected approach. Physical Review B, 2005, 71, .	1.1	86
38	Superconductivity from doping boron icosahedra. Physical Review B, 2004, 69, .	1.1	84
39	High- $T_c$ Superconductivity in Superhard Diamondlike BC <sub>5</sub> . Physical Review Letters, 2008, 101, 016401.	2.9	81
40	Intercalant and Intermolecular Phonon Assisted Superconductivity in K-Doped Picene. Physical Review Letters, 2011, 107, 137006.	2.9	79
41	Giant Nonadiabatic Effects in Layer Metals: Raman Spectra of Intercalated Graphite Explained. Physical Review Letters, 2008, 100, 226401.	2.9	75
42	Anharmonic effects in atomic hydrogen: Superconductivity and lattice dynamical stability. Physical Review B, 2016, 93, .	1.1	75
43	Intrinsic charge transfer gap in NiO from $K$ -edge x-ray absorption spectroscopy. Physical Review B, 2009, 79, .	1.1	72
44	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.	0.7	70
45	Anharmonic suppression of charge density waves in $HfNb_2S_7$ . Physical Review B, 2012, 86, .	1.1	66
46	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, .	1.1	66
47	Electronic band structure of Two-Dimensional $WS_2$ /Graphene van der Waals Heterostructures. Physical Review B, 2018, 97, .	1.1	63
48	Strong anharmonicity in the phonon spectra of PbTe and SnTe from first principles. Physical Review B, 2018, 97, .	1.1	63
49	Quantum Enhancement of Charge Density Wave in NbS <sub>2</sub> in the Two-Dimensional Limit. Nano Letters, 2019, 19, 3098-3103.	4.5	62
50	Projector augmented wave calculation of x-ray absorption spectra at the $L_{2,3}$ . Physical Review B, 2013, 87, .	1.1	59
51	Charge Fluctuations Close to Phase Separation in the Two-Dimensional $J_1$ Model. Physical Review Letters, 1998, 81, 5185-5188.	2.9	58
52	Possibility of superconductivity in graphite intercalated with alkaline earths investigated with density functional theory. Physical Review B, 2006, 74, .	1.1	57
53	Electronic structure of heavily doped graphene: The role of foreign atom states. Physical Review B, 2007, 76, .	1.1	57
54	Electronic and vibrational properties of $TiSe_2$ in the charge-density-wave phase from first principles. Physical Review B, 2015, 92, .	1.1	55

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55	Pressure and stress tensor of complex anharmonic crystals within the stochastic self-consistent harmonic approximation. <i>Physical Review B</i> , 2018, 98, .	1.1	56
56	Critical Role of the Exchange Interaction for the Electronic Structure and Charge-Density-Wave Formation in $\text{TiSe}_2$ . <i>Physical Review Letters</i> , 2017, 119, 176401.	2.9	55
57	Electron-phonon coupling and phonon self-energy in $\text{MgB}_2$ : Interpretation of $\text{MgB}_2$ Raman spectra. <i>Physical Review B</i> , 2005, 71, .	1.1	53
58	Phonon-Assisted Magnetic Mott-Insulating State in the Charge Density Wave Phase of Single-Layer $\text{TiTe}_2$ . <i>Physical Review Letters</i> , 2018, 121, 026401.	2.0	52
59	Magnetic gap opening in rhombohedral-stacked multilayer graphene from first principles. <i>Physical Review B</i> , 2017, 95, .	1.1	48
60	Anharmonic and non-adiabatic effects in $\text{MgB}_2$ : Implications for the isotope effect and interpretation of Raman spectra. <i>Physica C: Superconductivity and Its Applications</i> , 2007, 456, 38-44.	0.6	47
61	Electrical resistivity at large temperatures: Saturation and lack thereof. <i>Physical Review B</i> , 2002, 66, .	1.1	46
62	Dynamical properties of a strongly correlated model for quarter-filled layered organic molecular crystals. <i>Physical Review B</i> , 2003, 68, .	1.1	46
63	Electrochemical doping of few-layer $\text{ZrNCl}$ from first principles: Electronic and structural properties in field-effect configuration. <i>Physical Review B</i> , 2014, 89, .	1.1	46
64	Flat electronic bands in long sequences of rhombohedral-stacked graphene. <i>Physical Review B</i> , 2018, 97, .	1.1	46
65	Weak anharmonic effects in $\text{MgB}_2$ : A comparative inelastic x-ray scattering and Raman study. <i>Physical Review B</i> , 2007, 75, .	1.1	41
66	Metal-insulator transition and charge ordering in the extended Hubbard model at one-quarter filling. <i>Physical Review B</i> , 2002, 66, .	1.1	40
67	Black metal hydrogen above 360 GPa driven by proton quantum fluctuations. <i>Nature Physics</i> , 2021, 17, 63-67.	6.5	40
68	High-pressure phase diagram of hydrogen and deuterium sulfides from first principles: Structural and vibrational properties including quantum and anharmonic effects. <i>Physical Review B</i> , 2018, 97, .	1.1	38
69	Formation of hot-electron ensembles quasiequilibrated in momentum space by ultrafast momentum scattering of highly excited hot electrons photoinjected into the $\Gamma$ valley of GaAs. <i>Physical Review B</i> , 2016, 93, .	1.1	37
70	Weak Dimensionality Dependence and Dominant Role of Ionic Fluctuations in the Charge-Density-Wave Transition of $\text{NbSe}_2$ . <i>Physical Review Letters</i> , 2020, 125, 106101.	2.9	37
71	Electronic structure and magnetic properties of few-layer $\text{Cr}_2\text{Ge}_2\text{Te}_6$ : the key role of nonlocal electron-electron interaction effects. <i>2D Materials</i> , 2019, 6, 045042.	2.0	36
72	Search for high $T_c$ in layered structures: The case of $\text{LiB}$ . <i>Physical Review B</i> , 2007, 75, .	1.1	35

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73	Two-Dimensional Analysis of the Double-Resonant 2D Raman Mode in Bilayer Graphene. Physical Review Letters, 2014, 113, 187401.	2.9	35
74	Effect of electron doping on lattice instabilities in single-layer $\text{CuO}_2$ . Physical Review B, 2017, 95, .	1.1	26
75	Strong anharmonicity and high thermoelectric efficiency in high-temperature SnS from first principles. Physical Review B, 2019, 100, .	1.1	35
76	Polarized Resonant Inelastic X-Ray Scattering as an Ultrafine Probe of Excited States of $\text{La}_2\text{CuO}_4$ . Physical Review Letters, 2006, 96, 077006.	2.9	34
77	From antiferromagnetism to d-wave superconductivity in the two-dimensional $t$ - $J$ model. Physical Review B, 2000, 61, R11894-R11897.	1.1	30
78	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, .	1.1	30
79	Thermodynamic stabilities of ternary metal borides: An <i>ab initio</i> guide for synthesizing layered superconductors. Physical Review B, 2008, 78, .	1.1	29
80	Possible phase separation and weak localization in the absence of a charge-density wave in single-phase $\text{CuO}$ . Physical Review B, 2014, 89, .	1.1	28
81	van der Waals driven anharmonic melting of the 3D charge density wave in $\text{VSe}_2$ . Nature Communications, 2021, 12, 598.	5.8	28
82	Charge density wave and spin 1/2 insulating state in single layer $1\text{T-NbS}_2$ . 2D Materials, 2019, 6, 035041.	2.0	27
83	Anharmonic enhancement of superconductivity in metallic molecular $\text{C}_{60}$ hydrogen at high pressure: a first-principles study. Journal of Physics Condensed Matter, 2016, 28, 494001.	0.7	26
84	Violation of Ioffe-Regel condition but saturation of resistivity of the high- $T_c$ cuprates. Europhysics Letters, 2003, 61, 88-94.	0.7	25
85	Local and nonlocal electron-phonon couplings in $\text{K}_3\text{C}_6\text{O}_7$ picene and the effect of metallic screening. Physical Review B, 2012, 86, .	1.1	25
86	Anharmonicity and Doping Melt the Charge Density Wave in Single-Layer $\text{TiSe}_2$ . Nano Letters, 2020, 20, 4809-4815.	4.5	24
87	Understanding the Photomagnetic Behavior in Copper Octacyanomolybdates. Journal of Physical Chemistry A, 2012, 116, 8678-8683.	1.1	23
88	Density-functional calculation of static screening in two-dimensional materials: The long-wavelength dielectric function of graphene. Physical Review B, 2015, 91, .	1.1	21
89	Saturation of Electrical Resistivity in Metals at Large Temperatures. Physical Review Letters, 2001, 87, 266601.	2.9	20
90	Phonon softening in $\text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O}$ : Implications for the Fermi surface topology and the superconducting state. Physical Review B, 2006, 74, .	1.1	19

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91	First-principles determination of the Raman fingerprint of rhombohedral graphite. Physical Review Materials, 2017, 1, .	0.9	19
92	X-ray magnetic and natural circular dichroism from first principles: Calculation of $K$ - and $L$ -edge spectra. Physical Review B, 2017, 96, .	1.1	18
93	Misfit Layer Compounds: A Platform for Heavily Doped 2D Transition Metal Dichalcogenides. Advanced Functional Materials, 2021, 31, 2007706.	7.8	17
94	Theory of the thickness dependence of the charge density wave transition in 1 T-TiTe <sub>2</sub> . 2D Materials, 2020, 7, 045032.	2.0	17
95	Electronic structure of pristine and Ni-substituted $LaFeO_3$ from near edge x-ray absorption fine structure experiments and first-principles simulations. Physical	1.3	17
96	Maximum $T_c$ at the verge of a simultaneous order-disorder and lattice-softening transition in superconducting $CaC_6$ . Physical Review B, 2008, 78, .	1.1	16
97	Charge density waves go nano. Nature Nanotechnology, 2015, 10, 737-738.	15.6	16
98	Atomic and electronic structure of trilayer graphene/SiC(0001): Evidence of Strong Dependence on Stacking Sequence and charge transfer. Scientific Reports, 2016, 6, 33487.	1.6	16
99	Energy relaxation mechanism of hot-electron ensembles in GaAs: Theoretical and experimental study of its temperature dependence. Physical Review B, 2018, 97, .	1.1	16
100	Chiral Spin Texture in the Charge-Density-Wave Phase of the Correlated Metallic $Pb_{111}Tj$ . Scientific Reports, 2019, 9, 15487.	2.9	15
101	Neutron scattering study of the high-energy graphitic phonons in superconducting $CaC_6$ . Physical Review B, 2011, 84, .	1.1	14
102	Comparative study of the phonons in nonsuperconducting $BaC_6$ and superconducting $CaC_6$ using inelastic x-ray scattering. Physical Review B, 2011, 84, .	1.1	14
103	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.	2.9	14
104	Quantum effects in muon spin spectroscopy within the stochastic self-consistent harmonic approximation. Physical Review Materials, 2019, 3, .	0.9	13
105	Origin of superconductivity of $CaC_6$ and of other intercalated graphites. Physica Status Solidi (B): Basic Research, 2006, 243, 3458-3463.	0.7	12
106	Phonon dispersion and low-energy anomaly in $CaC_6$ inelastic neutron and x-ray scattering experiments. Physical Review B, 2010, 81, .	1.1	12
107	Superconductivity in metal-coated graphene. Physica Status Solidi (B): Basic Research, 2012, 249, 2544-2548.	0.7	12
108	Long-Range Rhombohedral-Stacked Graphene through Shear. Nano Letters, 2020, 20, 5017-5023.	4.5	12

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109	Gate-Tunable Magnetism and Giant Magnetoresistance in Suspended Rhombohedral-Stacked Few-Layer Graphene. Nano Letters, 2022, 22, 5094-5099.	4.5	12
110	Electronic thermal conductivity at high temperatures: Violation of the Wiedemann-Franz law in narrow-band metals. Physical Review B, 2006, 74, .	1.1	11
111	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.	1.3	10
112	Field-effect-driven half-metallic multilayer graphene. Physical Review B, 2018, 98, .	1.1	10
113	Thermal conductivity of Bi <sub>2</sub> Se <sub>3</sub> from bulk to thin films: Theory and experiment. Physical Review B, 2020, 101, .	1.1	10
114	Intrinsic Vibrational Angular Momentum from Nonadiabatic Effects in Noncollinear Magnetic Molecules. Physical Review Letters, 2021, 126, 225703.	2.9	10
115	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.	2.1	10
116	Light-Tunable Charge Density Wave Orders in $\text{MoTe}_2$ and $\text{WTe}_2$ Single Layers. Physical Review Letters, 2021, 127, 257401.	2.9	10
117	Determination of scattering time and of valley occupation in transition-metal dichalcogenides doped by field effect. Physical Review B, 2016, 93, .	1.1	9
118	2D Monolayer of the 1Tâ€™ Phase of Alloyed WSSe from Colloidal Synthesis. Journal of Physical Chemistry C, 2021, 125, 11058-11065.	1.5	9
119	Electric field exfoliation and high-TC superconductivity in field-effect hole-doped hydrogenated diamond (111). Applied Surface Science, 2019, 496, 143709.	3.1	8
120	Electronic structure of $\text{TiSe}_2$ from a quasi-self-consistent $G_0W_0$ approach. Physical Review B, 2021, 103, .	1.1	8
121	Lattice dynamics of photoexcited insulators from constrained density-functional perturbation theory. Physical Review B, 2021, 104, .	1.1	8
122	Publisher's Note: Electronic structure of heavily doped graphene: The role of foreign atom states [Phys. Rev. B <b>76</b> , 161406 (2007)]. Physical Review B, 2007, 76, .	1.1	7
123	Comment on "Electronic Structure of Superconducting $\text{KC}_8$ and Nonsuperconducting $\text{LiC}_6$ Graphite Intercalation Compounds: Evidence for a Graphene-Sheet-Driven Superconducting State". Physical Review Letters, 2012, 108, 149701; discussion 149702.	1.1	7
124	Comment on "Electronic Structure of Superconducting $\text{KC}_8$ and Nonsuperconducting $\text{LiC}_6$ Graphite Intercalation Compounds: Evidence for a Graphene-Sheet-Driven Superconducting State". Physical Review Letters, 2012, 108, 149701; discussion 149702.	2.9	7
125	Hybrid-functional electronic structure of multilayer graphene. Physical Review B, 2020, 101, .	1.1	7
126	Ab-initio energetics of graphite and multilayer graphene: stability of Bernal versus rhombohedral stacking. 2D Materials, 2021, 8, 035006.	2.0	7



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127	Spin susceptibility and electron-phonon coupling of two-dimensional materials by range-separated hybrid density functionals: Case study of $\text{Li}_x\text{Cu}_y\text{O}$ . Physical Review B, 2016, 94, .	1.1	5
128	High- $T_c$ superconductivity in weakly electron-doped HfNiCl. Physical Review B, 2017, 96, .	1.1	5
129	<i>Ab initio</i> study of the LiH phase diagram at extreme pressures and temperatures. Physical Review B, 2019, 99, .	1.1	5
130	Calandra and Mauri Reply. Physical Review Letters, 2014, 112, 049702.	2.9	4
131	Anharmonicity and the isotope effect in superconducting lithium at high pressures: A first-principles approach. Physical Review B, 2017, 96, .	1.1	4
132	Polar magnetic metallic state in few-layer $\text{BiFeO}_3$ . Physical Review B, 2021, 104, .	1.1	4
133	Charge density wave in single-layer Pb/Ge(111) driven by Pb-substrate exchange interaction. Physical Review B, 2021, 104, .	1.1	3
134	Multiple pre-edge structures in $\text{CuK}$ -edge x-ray absorption spectra of high- $T_c$ cuprates revealed by high-resolution x-ray absorption spectroscopy. Physical Review B, 2010, 81, .	1.1	2
135	Huge anharmonic effects in superconducting hydrides and transition metal dichalcogenides. Physica Status Solidi (B): Basic Research, 2014, 251, 2556-2562.	0.7	2
136	Theory of ultrafast magnetization of nonmagnetic semiconductors with localized conduction bands. Physical Review B, 2022, 105, .	1.1	1
137	High Pressure and Superconductivity: Intercalated Graphite $\text{C}_{60}$ as a Model System. NATO Science for Peace and Security Series B: Physics and Biophysics, 2010, , 407-418.	0.2	0
138	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.	0.3	0
139	Exchange Enhancement of the Electron-Phonon Interaction: The Case of Weakly Doped Two-Dimensional Multivalley Semiconductors. Journal of the Physical Society of Japan, 2018, 87, 041013.	0.7	0