Michele Lazzeri

List of Publications by Year
in descending order

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120 papers	48,643 citations	31902 53 h-index	18606 119 g-index
123 all docs	123 docs citations	123 times ranked	47189 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	Raman Spectrum of Graphene and Graphene Layers. Physical Review Letters, 2006, 97, 187401.	2.9	12,689
3	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	0.7	4,303
4	Structure and energetics of stoichiometricTiO2anatase surfaces. Physical Review B, 2001, 63, .	1.1	1,258
5	Breakdown of the adiabatic Bornâ€“Oppenheimer approximation in graphene. Nature Materials, 2007, 6, 198-201.	13.3	1,229
6	Kohn Anomalies and Electron-Phonon Interactions in Graphite. Physical Review Letters, 2004, 93, 185503.	2.9	779
7	Structure, Stability, Edge States, and Aromaticity of Graphene Ribbons. Physical Review Letters, 2008, 101, 096402.	2.9	582
8	Nonadiabatic Kohn Anomaly in a Doped Graphene Monolayer. Physical Review Letters, 2006, 97, 266407.	2.9	477
9	Theory of double-resonant Raman spectra in graphene: Intensity and line shape of defect-induced and two-phonon bands. Physical Review B, 2011, 84, .	1.1	476
10	Thermal Conductivity of Graphene and Graphite: Collective Excitations and Mean Free Paths. Nano Letters, 2014, 14, 6109-6114.	4.5	449
11	Optical phonons in carbon nanotubes: Kohn anomalies, Peierls distortions, and dynamic effects. Physical Review B, 2007, 75, .	1.1	418
12	Phonon Anharmonicities in Graphite and Graphene. Physical Review Letters, 2007, 99, 176802.	2.9	391
13	Phonon hydrodynamics in two-dimensional materials. Nature Communications, 2015, 6, 6400.	5.8	385
14	Phonon linewidths and electron-phonon coupling in graphite and nanotubes. Physical Review B, 2006, 73, .	1.1	335
15	First-Principles Calculation of Vibrational Raman Spectra in Large Systems: Signature of Small Rings in CrystallineSiO2. Physical Review Letters, 2003, 90, 036401.	2.9	313
16	Stress-Driven Reconstruction of an Oxide Surface: The AnataseTiO2(001)â^'(1Ã—4)Surface. Physical Review Letters, 2001, 87, 266105.	2.9	301
17	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, .	1.1	257
18	Electron Transport and Hot Phonons in Carbon Nanotubes. Physical Review Letters, 2005, 95, 236802.	2.9	250

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19	Clarâ€™s Theory, Ï€-Electron Distribution, and Geometry of Graphene Nanoribbons. Journal of the American Chemical Society, 2010, 132, 3440-3451.	6.6	219
20	Ab initiovariational approach for evaluating lattice thermal conductivity. Physical Review B, 2013, 88, .	1.1	199
21	Transport Properties of Graphene in the High-Current Limit. Physical Review Letters, 2009, 103, 076601.	2.9	188
22	Equilibrium isotopic fractionation in the kaolinite, quartz, water system: Prediction from first-principles density-functional theory. Geochimica Et Cosmochimica Acta, 2007, 71, 3170-3181.	1.6	180
23	Anharmonic properties from a generalized third-orderab initioapproach: Theory and applications to graphite and graphene. Physical Review B, 2013, 87, .	1.1	180
24	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.	1.6	173
25	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, .	1.1	170
26	Ab initiostudy of gap opening and screening effects in gated bilayer graphene. Physical Review B, 2009, 79, .	1.1	147
27	Single-atom vibrational spectroscopy in the scanning transmission electron microscope. Science, 2020, 367, 1124-1127.	6.0	143
28	Phonon Dispersion and Lifetimes inMgB2. Physical Review Letters, 2003, 90, 095506.	2.9	139
29	Doping in Carbon Nanotubes Probed by Raman and Transport Measurements. Physical Review Letters, 2007, 99, 136803.	2.9	135
30	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.	2.9	131
31	Structural control over equilibrium silicon and oxygen isotopic fractionation: A first-principles density-functional theory study. Chemical Geology, 2009, 258, 28-37.	1.4	128
32	Interstitial dinitrogen makesPtN2an insulating hard solid. Physical Review B, 2006, 73, .	1.1	125
33	Coupled dynamics of electrons and phonons in metallic nanotubes: Current saturation from hot-phonon generation. Physical Review B, 2006, 73, .	1.1	116
34	First-principles study of the OH-stretching modes of gibbsite. American Mineralogist, 2006, 91, 115-119.	0.9	115
35	Oxygen vacancy mediated adsorption and reactions of molecular oxygen on theTiO2(110)surface. Physical Review B, 2003, 68, .	1.1	113
36	Kohn anomalies and nonadiabaticity in doped carbon nanotubes. Physical Review B, 2007, 75, .	1.1	103

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37	Raman Fingerprint of Aligned Graphene/h-BN Superlattices. Nano Letters, 2013, 13, 5242-5246.	4.5	102
38	Anharmonic phonon frequency shift inMgB2. Physical Review B, 2003, 68, .	1.1	88
39	Structure and stability of graphene nanoribbons in oxygen, carbon dioxide, water, and ammonia. Physical Review B, 2010, 82, .	1.1	85
40	Doped Graphene as Tunable Electronâ"Phonon Coupling Material. Nano Letters, 2010, 10, 1172-1176.	4.5	84
41	First-principles study of OH-stretching modes in kaolinite, dickite, and nacrite. American Mineralogist, 2005, 90, 50-60.	0.9	83
42	Phonon surface mapping of graphite: Disentangling quasi-degenerate phonon dispersions. Physical Review B, 2009, 80, .	1.1	83
43	Current-voltage characteristics of graphene devices: Interplay between Zener-Klein tunneling and defects. Physical Review B, 2010, 82, .	1.1	78
44	Ab initioRaman spectrum of the normal and disorderedMgAl2O4spinel. Physical Review B, 2006, 74, .	1.1	77
45	Giant Nonadiabatic Effects in Layer Metals: Raman Spectra of Intercalated Graphite Explained. Physical Review Letters, 2008, 100, 226401.	2.9	75
46	A carbonate-fluoride defect model for carbonate-rich fluorapatite. American Mineralogist, 2013, 98, 1066-1069.	0.9	69
47	Line-broadening effects in the powder infrared spectrum of apatite. Physics and Chemistry of Minerals, 2011, 38, 111-122.	0.3	68
48	Anharmonicity of inner-OH stretching modes in hydrous phyllosilicates: assessment from first-principles frozen-phonon calculations. Physics and Chemistry of Minerals, 2007, 34, 621-625.	0.3	62
49	First-principles calculation of the infrared spectrum of hematite. American Mineralogist, 2008, 93, 1019-1027.	0.9	61
50	Hidden polymorphs drive vitrification in B2O3. Nature Materials, 2012, 11, 925-929.	13.3	60
51	Signature of the two-dimensional phonon dispersion in graphene probed by double-resonant Raman scattering. Physical Review B, 2013, 87, .	1.1	60
52	Surface modes in the infrared spectrum of hydrous minerals: the OH stretching modes of bayerite. Physics and Chemistry of Minerals, 2008, 35, 279-285.	0.3	55
53	First-principles calculation of H/D isotopic fractionation between hydrous minerals and water. Geochimica Et Cosmochimica Acta, 2010, 74, 3874-3882.	1.6	55
54	Theoretical infrared absorption coefficient of OH groups in minerals. American Mineralogist, 2008, 93, 950-953.	0.9	54

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55	First-principles study of the thermal expansion ofBe(101Â¯0). Physical Review B, 2002, 65, .	1.1	52
56	Ab initio resonant Raman spectra of diamond-like carbons. Diamond and Related Materials, 2005, 14, 1078-1083.	1.8	49
57	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.	0.6	47
58	Ab Initio Study of Be (0001) Surface Thermal Expansion. Physical Review Letters, 1998, 81, 2096-2099.	2.9	46
59	Nature of Hexagonal Silicon Forming via High-Pressure Synthesis: Nanostructured Hexagonal 4H Polytype. Nano Letters, 2018, 18, 5989-5995.	4.5	43
60	Elasticity of serpentines and extensive serpentinization in subduction zones. Geophysical Research Letters, 2007, 34, .	1.5	42
61	Pressure-induced phase transitions in amorphous and metastable crystalline germanium by Raman scattering, x-ray spectroscopy, andab initiocalculations. Physical Review B, 2009, 80, .	1.1	42
62	Weak anharmonic effects inMgB2: A comparative inelastic x-ray scattering and Raman study. Physical Review B, 2007, 75, .	1.1	41
63	Raman spectra of BN nanotubes:Ab initioand bond-polarizability model calculations. Physical Review B, 2005, 71, .	1.1	40
64	First-principles simulation of arsenate adsorption on the (1<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 397 Td (xmlns:mml="http:/ surface of hematite. Geochimica Et Cosmochimica Acta, 2012, 86, 182-195.	1.6	40
65	First-principles investigation of equilibrium isotopic fractionation of O- and Si-isotopes between refractory solids and gases in the solar nebula. Earth and Planetary Science Letters, 2012, 319-320, 118-127.	1.8	39
66	Probing the electrostatic environment of bilayer graphene using Raman spectra. Physical Review B, 2009, 80, .	1.1	38
67	Growth mechanism of silicene on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ag</mml:mi><mml:mo>(</mml:mo><mml:mn>111</mml:m by scanning tunneling microscopy measurements andab initiocalculations. Physical Review B, 2015, 92, .	1.1	38
68	Reduced partition function ratios of iron and oxygen in goethite. Geochimica Et Cosmochimica Acta, 2015, 151, 19-33.	1.6	38
69	Optical phonons of graphene and nanotubes. European Physical Journal: Special Topics, 2007, 148, 159-170.	1.2	35
70	Two-Dimensional Analysis of the Double-Resonant 2D Raman Mode in Bilayer Graphene. Physical Review Letters, 2014, 113, 187401.	2.9	35
71	Temperature evolution of infrared- and Raman-active phonons in graphite. Physical Review B, 2012, 86, .	1.1	34
72	First-principles study of the structural and isotopic properties of Al- and OH-bearing hematite. Geochimica Et Cosmochimica Acta, 2010, 74, 3948-3962.	1.6	32

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73	Raman spectrum of ammonia IV. Physical Review B, 2006, 74, .	1.1	31
74	Determining the atomic structure of the (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 712 Td (xmlns:mml="http://www.w3.org/19 first-principles calculations. Physical Review B, 2016, 94, .	1.1	27
75	Ab-initio dynamical properties of the Be(0001) surface. Surface Science, 1998, 402-404, 715-718.	0.8	26
76	First-principles modeling of sulfate incorporation and 34S/32S isotopic fractionation in different calcium carbonates. Chemical Geology, 2014, 374-375, 84-91.	1.4	26
77	Infrared spectroscopic properties of goethite: anharmonic broadening, long-range electrostatic effects and Al substitution. Physics and Chemistry of Minerals, 2014, 41, 289-302.	0.3	24
78	Experimental and theoretical study of the vibrational properties of diaspore (Î±-AlOOH). Physics and Chemistry of Minerals, 2012, 39, 93-102.	0.3	22
79	Flat Bands and Giant Light-Matter Interaction in Hexagonal Boron Nitride. Physical Review Letters, 2021, 127, 137401.	2.9	22
80	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.	1.6	21
81	Hydrodynamic Heat Transport Regime in Bismuth: A Theoretical Viewpoint. Physical Review Letters, 2018, 120, 075901.	2.9	21
82	Theoretical investigation of the anomalous equilibrium fractionation of multiple sulfur isotopes during adsorption. Earth and Planetary Science Letters, 2009, 284, 88-93.	1.8	20
83	Contribution of interstitial OH groups to the incorporation of water in forsterite. Physics and Chemistry of Minerals, 2014, 41, 105-114.	0.3	20
84	First-Principles Vibrational Electron Energy Loss Spectroscopy of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î²</mml:mi></mml:math> -Guanine. Physical Review Letters, 2017, 119, 027402.	2.9	19
85	High-order density-matrix perturbation theory. Physical Review B, 2003, 68, .	1.1	18
86	Ab initio study of Be surface dynamical properties. Surface Science, 2000, 454-456, 442-446.	0.8	17
87	Multilayer silicene: clear evidence of Ag-terminated bulk silicon. 2D Materials, 2017, 4, 025067.	2.0	17
88	Surface reconstructions of epitaxial MnAs films grown on GaAs(111)B. Physical Review B, 2006, 74, .	1.1	16
89	High-field transport in graphene: the impact of Zener tunneling. Journal of Physics Condensed Matter, 2015, 27, 164205.	0.7	16
90	Nanoscale mechanisms for the reduction of heat transport in bismuth. Physical Review B, 2016, 93, .	1.1	16

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91	Temperature dependence of X-ray absorption and nuclear magnetic resonance spectra: probing quantum vibrations of light elements in oxides. Physical Chemistry Chemical Physics, 2017, 19, 6246-6256.	1.3	16
92	Application of Raman spectroscopy to the study of graphitic carbons in the Earth Sciences. , 0, , 415-454.		16
93	Tuning of ZnSeâ€“GaAs band discontinuities in heterojunction diodes. Applied Physics Letters, 1996, 69, 3233-3235.	1.5	15
94	Theoretical Raman spectrum and anharmonicity of tetrahedral OH defects in hydrous forsterite. European Journal of Mineralogy, 2017, 29, 201-212.	0.4	15
95	Infrared reflectance, transmittance, and emittance spectra of MgO from first principles. Physical Review B, 2018, 98, .	1.1	15
96	Surface oscillatory thermal expansion:â€ƒMg(101Â¯0). Physical Review B, 2001, 63, .	1.1	14
97	New constraints on Xe incorporation mechanisms in olivine from first-principles calculations. Geochimica Et Cosmochimica Acta, 2018, 222, 146-155.	1.6	14
98	Structure and stability of silicene on Ag(111) reconstructions from grazing incidence x-ray diffraction and density functional theory. Physical Review B, 2019, 99, .	1.1	14
99	Boosting Electronic Transport in Carbon Nanotubes by Isotopic Disorder. Physical Review Letters, 2009, 102, 196801.	2.9	13
100	Infrared spectroscopic study of sulfate-bearing calcite from deep-sea bamboo coral. European Journal of Mineralogy, 2017, 29, 397-408.	0.4	13
101	Thermal transport in isotopically disordered carbon nanotubes: a comparison between Greenâ€™s functions and Boltzmann approaches. Journal of Physics Condensed Matter, 2009, 21, 245302.	0.7	11
102	Theoretical study of the local charge compensation and spectroscopic properties of B-type carbonate defects in apatite. Physics and Chemistry of Minerals, 2014, 41, 347-359.	0.3	11
103	The mechanism for the stabilization and surfactant properties of epitaxial silicene. Nanoscale, 2018, 10, 2291-2300.	2.8	11
104	Formation of silicene on silver: Strong interaction between Ag and Si. Physica Status Solidi (B): Basic Research, 2016, 253, 206-217.	0.7	10
105	The thermodynamic stability and simulated STM images of graphene nanoribbons. Physica Status Solidi (B): Basic Research, 2009, 246, 2586-2591.	0.7	9
106	Zener tunneling in the electrical transport of quasimetallic carbon nanotubes. Physical Review B, 2012, 86, .	1.1	9
107	Carbon-Based Nanoscience. Elements, 2014, 10, 447-452.	0.5	8
108	Structure, reactivity and spectroscopic properties of minerals from lateritic soils: insights from ab initio calculations. European Journal of Soil Science, 2007, 58, 870-881.	1.8	6

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109	Fermi resonance in the Raman spectrum of graphene. Physical Review B, 2020, 102, .	1.1	6
110	Exciton and Phonon Radiative Linewidths in Monolayer Boron Nitride. Physical Review X, 2022, 12, .	2.8	5
111	Kohn Anomalies in Graphite and Nanotubes. Materials Research Society Symposia Proceedings, 2004, 858, 283.	0.1	4
112	Line-broadening and anharmonic effects in the attenuated total reflectance infrared spectra of calcite. European Journal of Mineralogy, 2019, 31, 73-81.	0.4	4
113	Ultrafast nonlinear phonon response of few-layer hexagonal boron nitride. Physical Review B, 2021, 104, .	1.1	4
114	Electrical characterization of engineered ZnSeî—¸GaAs heterojunction diodes. Journal of Crystal Growth, 1997, 175-176, 603-607.	0.7	3
115	Publisherâ€™s Note: Electron Transport and Hot Phonons in Carbon Nanotubes [Phys. Rev. Lett.95, 236802 (2005)]. Physical Review Letters, 2005, 95, .	2.9	3
116	Kohn Anomalies and Electron-Phonon Coupling in Carbon Nanotubes. AIP Conference Proceedings, 2005, , .	0.3	2
117	Breakdown of the adiabatic approximation in a doped graphene monolayer and in metallic carbon nanotubes. Physica Status Solidi (B): Basic Research, 2007, 244, 4118-4123.	0.7	2
118	Modeling Vibrational EELS: From Bulk to Point Defects. Microscopy and Microanalysis, 2020, 26, 946-947.	0.2	1
119	Assessing temperature effects on multipole contributions and angular dependence in core-level spectroscopies. Physical Review B, 2021, 104, .	1.1	1
120	First-Principles Modeling of Vibrational Electron Energy Loss Spectra. Microscopy and Microanalysis, 2019, 25, 602-603.	0.2	0