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	Exciton and Phonon Radiative Linewidths in Monolayer Boron Nitride. Physical Review X, 2022, 12, .	2.8	5
2	Assessing temperature effects on multipole contributions and angular dependence in core-level spectroscopies. Physical Review B, 2021, 104, .	1.1	1
3	Flat Bands and Giant Light-Matter Interaction in Hexagonal Boron Nitride. Physical Review Letters, 2021, 127, 137401.	2.9	22
4	Ultrafast nonlinear phonon response of few-layer hexagonal boron nitride. Physical Review B, 2021, 104, .	1.1	4
5	Modeling Vibrational EELS: From Bulk to Point Defects. Microscopy and Microanalysis, 2020, 26, 946-947.	0.2	1
6	Fermi resonance in the Raman spectrum of graphene. Physical Review B, 2020, 102, .	1.1	6
7	Single-atom vibrational spectroscopy in the scanning transmission electron microscope. Science, 2020, 367, 1124-1127.	6.0	143
8	First-Principles Modeling of Vibrational Electron Energy Loss Spectra. Microscopy and Microanalysis, 2019, 25, 602-603.	0.2	0
9	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
10	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
11	Hydrodynamic Heat Transport Regime in Bismuth: A Theoretical Viewpoint. Physical Review Letters, 2018, 120, 075901.	2.9	21
12	The mechanism for the stabilization and surfactant properties of epitaxial silicene. Nanoscale, 2018, 10, 2291-2300.	2.8	11
13	New constraints on Xe incorporation mechanisms in olivine from first-principles calculations. Geochimica Et Cosmochimica Acta, 2018, 222, 146-155.	1.6	14
14	Infrared reflectance, transmittance, and emittance spectra of MgO from first principles. Physical Review B, 2018, 98, .	1.1	15
15	Nature of Hexagonal Silicon Forming via High-Pressure Synthesis: Nanostructured Hexagonal 4H Polytype. Nano Letters, 2018, 18, 5989-5995.	4.5	43
16	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
17	Theoretical Raman spectrum and anharmonicity of tetrahedral OH defects in hydrous forsterite. European Journal of Mineralogy, 2017, 29, 201-212.	0.4	15
18	Infrared spectroscopic study of sulfate-bearing calcite from deep-sea bamboo coral. European Journal of Mineralogy, 2017, 29, 397-408.	0.4	13

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19	Multilayer silicene: clear evidence of Ag-terminated bulk silicon. 2D Materials, 2017, 4, 025067.	2.0	17
20	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	0.7	4,303
21	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
22	Formation of silicene on silver: Strong interaction between Ag and Si. Physica Status Solidi (B): Basic Research, 2016, 253, 206-217.	0.7	10
23	Nanoscale mechanisms for the reduction of heat transport in bismuth. Physical Review B, 2016, 93, .	1.1	16
24	Determining the atomic structure of the (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 552 Td (xmlns:mml="http://www.w3.org/19 first-principles calculations. Physical Review B, 2016, 94, .	1.1	27
25	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
26	Phonon hydrodynamics in two-dimensional materials. Nature Communications, 2015, 6, 6400.	5.8	385
27	High-field transport in graphene: the impact of Zener tunneling. Journal of Physics Condensed Matter, 2015, 27, 164205.	0.7	16
28	Reduced partition function ratios of iron and oxygen in goethite. Geochimica Et Cosmochimica Acta, 2015, 151, 19-33.	1.6	38
29	Carbon-Based Nanoscience. Elements, 2014, 10, 447-452.	0.5	8
30	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
31	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
32	Contribution of interstitial OH groups to the incorporation of water in forsterite. Physics and Chemistry of Minerals, 2014, 41, 105-114.	0.3	20
33	Thermal Conductivity of Graphene and Graphite: Collective Excitations and Mean Free Paths. Nano Letters, 2014, 14, 6109-6114.	4.5	449
34	Two-Dimensional Analysis of the Double-Resonant 2D Raman Mode in Bilayer Graphene. Physical Review Letters, 2014, 113, 187401.	2.9	35
35	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
36	Ab initiovariational approach for evaluating lattice thermal conductivity. Physical Review B, 2013, 88, .	1.1	199

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37	Raman Fingerprint of Aligned Graphene/h-BN Superlattices. Nano Letters, 2013, 13, 5242-5246.	4.5	102
38	Signature of the two-dimensional phonon dispersion in graphene probed by double-resonant Raman scattering. Physical Review B, 2013, 87, .	1.1	60
39	Anharmonic properties from a generalized third-orderab initioapproach: Theory and applications to graphite and graphene. Physical Review B, 2013, 87, .	1.1	180
40	A carbonate-fluoride defect model for carbonate-rich fluorapatite. American Mineralogist, 2013, 98, 1066-1069.	0.9	69
41	Zener tunneling in the electrical transport of quasimetallic carbon nanotubes. Physical Review B, 2012, 86, .	1.1	9
42	Hidden polymorphs drive vitrification in B2O3. Nature Materials, 2012, 11, 925-929.	13.3	60
43	Temperature evolution of infrared- and Raman-active phonons in graphite. Physical Review B, 2012, 86, .	1.1	34
44	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
45	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
46	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
47	Experimental and theoretical study of the vibrational properties of diaspore (Î±-AlOOH). Physics and Chemistry of Minerals, 2012, 39, 93-102.	0.3	22
48	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
49	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
50	Line-broadening effects in the powder infrared spectrum of apatite. Physics and Chemistry of Minerals, 2011, 38, 111-122.	0.3	68
51	Structure and stability of graphene nanoribbons in oxygen, carbon dioxide, water, and ammonia. Physical Review B, 2010, 82, .	1.1	85
52	Current-voltage characteristics of graphene devices: Interplay between Zener-Klein tunneling and defects. Physical Review B, 2010, 82, .	1.1	78
53	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
54	First-principles calculation of H/D isotopic fractionation between hydrous minerals and water. Geochimica Et Cosmochimica Acta, 2010, 74, 3874-3882.	1.6	55

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55	Clarâ€™s Theory, Ï€-Electron Distribution, and Geometry of Graphene Nanoribbons. Journal of the American Chemical Society, 2010, 132, 3440-3451.	6.6	219
56	Doped Graphene as Tunable Electronâ^'Phonon Coupling Material. Nano Letters, 2010, 10, 1172-1176.	4.5	84
57	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
58	Probing the electrostatic environment of bilayer graphene using Raman spectra. Physical Review B, 2009, 80, .	1.1	38
59	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
60	The thermodynamic stability and simulated STM images of graphene nanoribbons. Physica Status Solidi (B): Basic Research, 2009, 246, 2586-2591.	0.7	9
61	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
62	Phonon surface mapping of graphite: Disentangling quasi-degenerate phonon dispersions. Physical Review B, 2009, 80, .	1.1	83
63	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
64	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
65	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
66	Boosting Electronic Transport in Carbon Nanotubes by Isotopic Disorder. Physical Review Letters, 2009, 102, 196801.	2.9	13
67	Ab initiostudy of gap opening and screening effects in gated bilayer graphene. Physical Review B, 2009, 79, .	1.1	147
68	Transport Properties of Graphene in the High-Current Limit. Physical Review Letters, 2009, 103, 076601.	2.9	188
69	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
70	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
71	Structure, Stability, Edge States, and Aromaticity of Graphene Ribbons. Physical Review Letters, 2008, 101, 096402.	2.9	582
72	Theoretical infrared absorption coefficient of OH groups in minerals. American Mineralogist, 2008, 93, 950-953.	0.9	54

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73	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
74	First-principles calculation of the infrared spectrum of hematite. American Mineralogist, 2008, 93, 1019-1027.	0.9	61
75	Giant Nonadiabatic Effects in Layer Metals: Raman Spectra of Intercalated Graphite Explained. Physical Review Letters, 2008, 100, 226401.	2.9	75
76	Kohn anomalies and nonadiabaticity in doped carbon nanotubes. Physical Review B, 2007, 75, .	1.1	103
77	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
78	Optical phonons in carbon nanotubes: Kohn anomalies, Peierls distortions, and dynamic effects. Physical Review B, 2007, 75, .	1.1	418
79	Weak anharmonic effects inMgB2: A comparative inelastic x-ray scattering and Raman study. Physical Review B, 2007, 75, .	1.1	41
80	Doping in Carbon Nanotubes Probed by Raman and Transport Measurements. Physical Review Letters, 2007, 99, 136803.	2.9	135
81	Elasticity of serpentines and extensive serpentinization in subduction zones. Geophysical Research Letters, 2007, 34, .	1.5	42
82	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
83	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
84	Breakdown of the adiabatic Bornâ€“Oppenheimer approximation in graphene. Nature Materials, 2007, 6, 198-201.	13.3	1,229
85	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
86	Phonon Anharmonicities in Graphite and Graphene. Physical Review Letters, 2007, 99, 176802.	2.9	391
87	Optical phonons of graphene and nanotubes. European Physical Journal: Special Topics, 2007, 148, 159-170.	1.2	35
88	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
89	Surface reconstructions of epitaxial MnAs films grown on GaAs(111)B. Physical Review B, 2006, 74, .	1.1	16
90	Phonon linewidths and electron-phonon coupling in graphite and nanotubes. Physical Review B, 2006, 73, .	1.1	335

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91	Nonadiabatic Kohn Anomaly in a Doped Graphene Monolayer. Physical Review Letters, 2006, 97, 266407.	2.9	477
92	Raman Spectrum of Graphene and Graphene Layers. Physical Review Letters, 2006, 97, 187401.	2.9	12,689
93	First-principles study of the OH-stretching modes of gibbsite. American Mineralogist, 2006, 91, 115-119.	0.9	115
94	Raman spectrum of ammonia IV. Physical Review B, 2006, 74, .	1.1	31
95	Ab initioRaman spectrum of the normal and disorderedMgAl2O4spinel. Physical Review B, 2006, 74, .	1.1	77
96	Coupled dynamics of electrons and phonons in metallic nanotubes: Current saturation from hot-phonon generation. Physical Review B, 2006, 73, .	1.1	116
97	Interstitial dinitrogen makesPtN2an insulating hard solid. Physical Review B, 2006, 73, .	1.1	125
98	Kohn Anomalies and Electron-Phonon Coupling in Carbon Nanotubes. AIP Conference Proceedings, 2005, , .	0.3	2
99	Raman spectra of BN nanotubes:Ab initioand bond-polarizability model calculations. Physical Review B, 2005, 71, .	1.1	40
100	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
101	First-principles study of OH-stretching modes in kaolinite, dickite, and nacrite. American Mineralogist, 2005, 90, 50-60.	0.9	83
102	Electron Transport and Hot Phonons in Carbon Nanotubes. Physical Review Letters, 2005, 95, 236802.	2.9	250
103	Ab initio resonant Raman spectra of diamond-like carbons. Diamond and Related Materials, 2005, 14, 1078-1083.	1.8	49
104	Kohn Anomalies in Graphite and Nanotubes. Materials Research Society Symposia Proceedings, 2004, 858, 283.	0.1	4
105	Kohn Anomalies and Electron-Phonon Interactions in Graphite. Physical Review Letters, 2004, 93, 185503.	2.9	779
106	Phonon Dispersion and Lifetimes inMgB2. Physical Review Letters, 2003, 90, 095506.	2.9	139
107	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
108	Oxygen vacancy mediated adsorption and reactions of molecular oxygen on theTiO2(110)surface. Physical Review B, 2003, 68, .	1.1	113

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109	Anharmonic phonon frequency shift inMgB2. Physical Review B, 2003, 68, .	1.1	88
110	High-order density-matrix perturbation theory. Physical Review B, 2003, 68, .	1.1	18
111	First-principles study of the thermal expansion ofBe(101Â¯0). Physical Review B, 2002, 65, .	1.1	52
112	Stress-Driven Reconstruction of an Oxide Surface: The AnataseTiO2(001)âˆ'(1Ã—4)Surface. Physical Review Letters, 2001, 87, 266105.	2.9	301
113	Structure and energetics of stoichiometricTiO2anatase surfaces. Physical Review B, 2001, 63, .	1.1	1,258
114	Surface oscillatory thermal expansion:â€ƒMg(101Â¯0). Physical Review B, 2001, 63, .	1.1	14
115	Ab initio study of Be surface dynamical properties. Surface Science, 2000, 454-456, 442-446.	0.8	17
116	Ab-initio dynamical properties of the Be(0001) surface. Surface Science, 1998, 402-404, 715-718.	0.8	26
117	Ab Initio Study of Be (0001) Surface Thermal Expansion. Physical Review Letters, 1998, 81, 2096-2099.	2.9	46
118	Electrical characterization of engineered ZnSeî—¸GaAs heterojunction diodes. Journal of Crystal Growth, 1997, 175-176, 603-607.	0.7	3
119	Tuning of ZnSeâ€“GaAs band discontinuities in heterojunction diodes. Applied Physics Letters, 1996, 69, 3233-3235.	1.5	15
120	Application of Raman spectroscopy to the study of graphitic carbons in the Earth Sciences. , 0, , 415-454.		16