Michele Lazzeri

List of Publications by Citations

117 papers	38,148 citations	50 h-index	123 g-index
123 ext. papers	43,321 ext. citations	5 avg, IF	6.72 L-index

#	Paper	IF	Citations
117	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. *Journal of Physics Condensed Matter*, **2009**, 21, 395502	1.8	13251
116	Raman spectrum of graphene and graphene layers. *Physical Review Letters*, **2006**, 97, 187401	7.4	11029
115	Advanced capabilities for materials modelling with Quantum ESPRESSO. *Journal of Physics Condensed Matter*, **2017**, 29, 465901	1.8	2275
114	Structure and energetics of stoichiometric TiO2 anatase surfaces. *Physical Review B*, **2001**, 63,	3.3	1143
113	Breakdown of the adiabatic Born-Oppenheimer approximation in graphene. *Nature Materials*, **2007**, 6, 198-201	27	1077
112	Kohn anomalies and electron-phonon interactions in graphite. *Physical Review Letters*, **2004**, 93, 185503	7.4	709
111	Structure, stability, edge states, and aromaticity of graphene ribbons. *Physical Review Letters*, **2008**, 101, 096402	7.4	521
110	Nonadiabatic Kohn anomaly in a doped graphene monolayer. *Physical Review Letters*, **2006**, 97, 266407	7.4	430
109	Theory of double-resonant Raman spectra in graphene: Intensity and line shape of defect-induced and two-phonon bands. *Physical Review B*, **2011**, 84,	3.3	409
108	Optical phonons in carbon nanotubes: Kohn anomalies, Peierls distortions, and dynamic effects. *Physical Review B*, **2007**, 75,	3.3	393
107	Thermal conductivity of graphene and graphite: collective excitations and mean free paths. *Nano Letters*, **2014**, 14, 6109-14	11.5	353
106	Phonon anharmonicities in graphite and graphene. *Physical Review Letters*, **2007**, 99, 176802	7.4	327
105	Phonon linewidths and electron-phonon coupling in graphite and nanotubes. *Physical Review B*, **2006**, 73,	3.3	290
104	Phonon hydrodynamics in two-dimensional materials. *Nature Communications*, **2015**, 6, 6400	17.4	282
103	Stress-driven reconstruction of an oxide surface: the anatase TiO(2)(001)-(1 x 4) surface. *Physical Review Letters*, **2001**, 87, 266105	7.4	274
102	First-principles calculation of vibrational Raman spectra in large systems: signature of small rings in crystalline SiO2. *Physical Review Letters*, **2003**, 90, 036401	7.4	266
101	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,	3.3	237

100	Electron transport and hot phonons in carbon nanotubes. *Physical Review Letters*, **2005**, 95, 236802	7.4	224
99	Clar's theory, pi-electron distribution, and geometry of graphene nanoribbons. *Journal of the American Chemical Society*, **2010**, 132, 3440-51	16.4	194
98	Transport properties of graphene in the high-current limit. *Physical Review Letters*, **2009**, 103, 076601	7.4	177
97	Ab initio variational approach for evaluating lattice thermal conductivity. *Physical Review B*, **2013**, 88,	3.3	164
96	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,	3.3	152
95	Equilibrium isotopic fractionation in the kaolinite, quartz, water system: Prediction from first-principles density-functional theory. *Geochimica Et Cosmochimica Acta*, **2007**, 71, 3170-3181	5.5	148
94	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	5.5	145
93	Anharmonic properties from a generalized third-order ab initio approach: Theory and applications to graphite and graphene. *Physical Review B*, **2013**, 87,	3.3	141
92	Ab initio study of gap opening and screening effects in gated bilayer graphene. *Physical Review B*, **2009**, 79,	3.3	134
91	Phonon dispersion and lifetimes in MgB2. *Physical Review Letters*, **2003**, 90, 095506	7.4	126
90	Doping in carbon nanotubes probed by Raman and transport measurements. *Physical Review Letters*, **2007**, 99, 136803	7.4	123
89	Boroxol Rings in Liquid and Vitreous B2O3 from First Principles. *Physical Review Letters*, **2008**, 101, 065504	7.4	118
88	Interstitial dinitrogen makes PtN2 an insulating hard solid. *Physical Review B*, **2006**, 73,	3.3	118
87	Structural control over equilibrium silicon and oxygen isotopic fractionation: A first-principles density-functional theory study. *Chemical Geology*, **2009**, 258, 28-37	4.2	108
86	Oxygen vacancy mediated adsorption and reactions of molecular oxygen on the TiO2(110) surface. *Physical Review B*, **2003**, 68,	3.3	99
85	Coupled dynamics of electrons and phonons in metallic nanotubes: Current saturation from hot-phonon generation. *Physical Review B*, **2006**, 73,	3.3	98
84	Kohn anomalies and nonadiabaticity in doped carbon nanotubes. *Physical Review B*, **2007**, 75,	3.3	96
83	First-principles study of the OH-stretching modes of gibbsite. *American Mineralogist*, **2006**, 91, 115-119	2.9	95

82	Raman fingerprint of aligned graphene/h-BN superlattices. *Nano Letters*, **2013**, 13, 5242-6	11.5	83
81	Anharmonic phonon frequency shift in MgB2. *Physical Review B*, **2003**, 68,	3.3	79
80	Structure and stability of graphene nanoribbons in oxygen, carbon dioxide, water, and ammonia. *Physical Review B*, **2010**, 82,	3.3	78
79	Doped graphene as tunable electron-phonon coupling material. *Nano Letters*, **2010**, 10, 1172-6	11.5	76
78	Phonon surface mapping of graphite: Disentangling quasi-degenerate phonon dispersions. *Physical Review B*, **2009**, 80,	3.3	75
77	Single-atom vibrational spectroscopy in the scanning transmission electron microscope. *Science*, **2020**, 367, 1124-1127	33.3	73
76	Current-voltage characteristics of graphene devices: Interplay between Zener-Klein tunneling and defects. *Physical Review B*, **2010**, 82,	3.3	67
75	Giant nonadiabatic effects in layer metals: raman spectra of intercalated graphite explained. *Physical Review Letters*, **2008**, 100, 226401	7.4	63
74	Ab initio Raman spectrum of the normal and disordered MgAl2O4 spinel. *Physical Review B*, **2006**, 74,	3.3	62
73	Line-broadening effects in the powder infrared spectrum of apatite. *Physics and Chemistry of Minerals*, **2011**, 38, 111-122	1.6	60
72	First-principles study of OH-stretching modes in kaolinite, dickite, and nacrite. *American Mineralogist*, **2005**, 90, 50-60	2.9	58
71	Letter. A carbonate-fluoride defect model for carbonate-rich fluorapatite. *American Mineralogist*, **2013**, 98, 1066-1069	2.9	53
70	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	1.6	53
69	Hidden polymorphs drive vitrification in B2O3. *Nature Materials*, **2012**, 11, 925-9	27	51
68	Signature of the two-dimensional phonon dispersion in graphene probed by double-resonant Raman scattering. *Physical Review B*, **2013**, 87,	3.3	50
67	First-principles study of the thermal expansion of Be(101□0). *Physical Review B*, **2002**, 65,	3.3	47
66	Surface modes in the infrared spectrum of hydrous minerals: the OH stretching modes of bayerite. *Physics and Chemistry of Minerals*, **2008**, 35, 279-285	1.6	46
65	Ab initio resonant Raman spectra of diamond-like carbons. *Diamond and Related Materials*, **2005**, 14, 1078-1083	3.5	45

64	Ab Initio Study of Be (0001) Surface Thermal Expansion. *Physical Review Letters*, **1998**, 81, 2096-2099	7.4	44
63	First-principles calculation of H/D isotopic fractionation between hydrous minerals and water. *Geochimica Et Cosmochimica Acta*, **2010**, 74, 3874-3882	5.5	42
62	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	1.3	42
61	Probing the electrostatic environment of bilayer graphene using Raman spectra. *Physical Review B*, **2009**, 80,	3.3	36
60	Raman spectra of BN nanotubes: Ab initio and bond-polarizability model calculations. *Physical Review B*, **2005**, 71,	3.3	36
59	First-principles simulation of arsenate adsorption on the (1. *Geochimica Et Cosmochimica Acta*, **2012**, 86, 182-195	5.5	35
58	Pressure-induced phase transitions in amorphous and metastable crystalline germanium by Raman scattering, x-ray spectroscopy, and ab initio calculations. *Physical Review B*, **2009**, 80,	3.3	35
57	Elasticity of serpentines and extensive serpentinization in subduction zones. *Geophysical Research Letters*, **2007**, 34, n/a-n/a	4.9	35
56	Weak anharmonic effects in MgB2: A comparative inelastic x-ray scattering and Raman study. *Physical Review B*, **2007**, 75,	3.3	35
55	Theoretical infrared absorption coefficient of OH groups in minerals. *American Mineralogist*, **2008**, 93, 950-953	2.9	33
54	First-principles calculation of the infrared spectrum of hematite. *American Mineralogist*, **2008**, 93, 1019-1027	2.9	32
53	Growth mechanism of silicene on Ag(111) determined by scanning tunneling microscopy measurements and ab initio calculations. *Physical Review B*, **2015**, 92,	3.3	31
52	Temperature evolution of infrared- and Raman-active phonons in graphite. *Physical Review B*, **2012**, 86,	3.3	31
51	Reduced partition function ratios of iron and oxygen in goethite. *Geochimica Et Cosmochimica Acta*, **2015**, 151, 19-33	5.5	30
50	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	5.3	30
49	Optical phonons of graphene and nanotubes. *European Physical Journal: Special Topics*, **2007**, 148, 159-170	2.3	29
48	Raman spectrum of ammonia IV. *Physical Review B*, **2006**, 74,	3.3	29
47	Two-dimensional analysis of the double-resonant 2D Raman mode in bilayer graphene. *Physical Review Letters*, **2014**, 113, 187401	7.4	28

46	Ab-initio dynamical properties of the Be(0001) surface. *Surface Science*, **1998**, 402-404, 715-718	1.8	26
45	Nature of Hexagonal Silicon Forming via High-Pressure Synthesis: Nanostructured Hexagonal 4H Polytype. *Nano Letters*, **2018**, 18, 5989-5995	11.5	24
44	First-principles study of the structural and isotopic properties of Al- and OH-bearing hematite. *Geochimica Et Cosmochimica Acta*, **2010**, 74, 3948-3962	5.5	22
43	Determining the atomic structure of the (4□4) silicene layer on Ag(111) by combined grazing-incidence x-ray diffraction measurements and first-principles calculations. *Physical Review B* , **2016**, 94,	3.3	20
42	Theoretical investigation of the anomalous equilibrium fractionation of multiple sulfur isotopes during adsorption. *Earth and Planetary Science Letters*, **2009**, 284, 88-93	5.3	20
41	First-principles modeling of sulfate incorporation and 34S/32S isotopic fractionation in different calcium carbonates. *Chemical Geology*, **2014**, 374-375, 84-91	4.2	19
40	Infrared spectroscopic properties of goethite: anharmonic broadening, long-range electrostatic effects and Al substitution. *Physics and Chemistry of Minerals*, **2014**, 41, 289-302	1.6	19
39	Comment on □New data on equilibrium iron isotope fractionation among sulfides: Constraints on mechanisms of sulfide formation in hydrothermal and igneous systems□by V.B. Polyakov and D.M. Soultanov. *Geochimica Et Cosmochimica Acta*, **2012**, 87, 356-359	5.5	17
38	Ab initio study of Be surface dynamical properties. *Surface Science*, **2000**, 454-456, 442-446	1.8	17
37	Contribution of interstitial OH groups to the incorporation of water in forsterite. *Physics and Chemistry of Minerals*, **2014**, 41, 105-114	1.6	16
36	High-order density-matrix perturbation theory. *Physical Review B*, **2003**, 68,	3.3	16
35	Multilayer silicene: clear evidence of Ag-terminated bulk silicon. *2D Materials*, **2017**, 4, 025067	5.9	15
34	Hydrodynamic Heat Transport Regime in Bismuth: A Theoretical Viewpoint. *Physical Review Letters*, **2018**, 120, 075901	7.4	15
33	First-Principles Vibrational Electron Energy Loss Spectroscopy of □Guanine. *Physical Review Letters* , **2017**, 119, 027402	7.4	15
32	Surface reconstructions of epitaxial MnAs films grown on GaAs(111)B. *Physical Review B*, **2006**, 74,	3.3	15
31	Nanoscale mechanisms for the reduction of heat transport in bismuth. *Physical Review B*, **2016**, 93,	3.3	14
30	Experimental and theoretical study of the vibrational properties of diaspore (□AlOOH). *Physics and Chemistry of Minerals*, **2012**, 39, 93-102	1.6	14
29	Tuning of ZnSe□GaAs band discontinuities in heterojunction diodes. *Applied Physics Letters*, **1996**, 69, 3233-3235	3.4	14

28	Boosting electronic transport in carbon nanotubes by isotopic disorder. *Physical Review Letters*, **2009**, 102, 196801	7.4	13
27	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	3.6	12
26	High-field transport in graphene: the impact of Zener tunneling. *Journal of Physics Condensed Matter*, **2015**, 27, 164205	1.8	12
25	New constraints on Xe incorporation mechanisms in olivine from first-principles calculations. *Geochimica Et Cosmochimica Acta*, **2018**, 222, 146-155	5.5	12
24	Theoretical Raman spectrum and anharmonicity of tetrahedral OH defects in hydrous forsterite. *European Journal of Mineralogy*, **2017**, 29, 201-212	2.2	11
23	Thermal transport in isotopically disordered carbon nanotubes: a comparison between Green's functions and Boltzmann approaches. *Journal of Physics Condensed Matter*, **2009**, 21, 245302	1.8	11
22	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	1.6	10
21	Surface oscillatory thermal expansion: Mg(101□0). *Physical Review B*, **2001**, 63,	3.3	10
20	The thermodynamic stability and simulated STM images of graphene nanoribbons. *Physica Status Solidi (B): Basic Research*, **2009**, 246, 2586-2591	1.3	9
19	Structure and stability of silicene on Ag(111) reconstructions from grazing incidence x-ray diffraction and density functional theory. *Physical Review B*, **2019**, 99,	3.3	8
18	The mechanism for the stabilization and surfactant properties of epitaxial silicene. *Nanoscale*, **2018**, 10, 2291-2300	7.7	8
17	Formation of silicene on silver: Strong interaction between Ag and Si. *Physica Status Solidi (B): Basic Research*, **2016**, 253, 206-217	1.3	8
16	Infrared spectroscopic study of sulfate-bearing calcite from deep-sea bamboo coral. *European Journal of Mineralogy*, **2017**, 29, 397-408	2.2	7
15	Application of Raman spectroscopy to the study of graphitic carbons in the Earth Sciences415-454		7
14	Carbon-Based Nanoscience. *Elements*, **2014**, 10, 447-452	3.8	6
13	Zener tunneling in the electrical transport of quasimetallic carbon nanotubes. *Physical Review B*, **2012**, 86,	3.3	6
12	Infrared reflectance, transmittance, and emittance spectra of MgO from first principles. *Physical Review B*, **2018**, 98,	3.3	6
11	Structure, reactivity and spectroscopic properties of minerals from lateritic soils: insights from ab initio calculations. *European Journal of Soil Science*, **2007**, 58, 870-881	3.4	5

10	Flat Bands and Giant Light-Matter Interaction in Hexagonal Boron Nitride. *Physical Review Letters*, **2021**, 127, 137401	7.4	5
9	Kohn Anomalies in Graphite and Nanotubes. *Materials Research Society Symposia Proceedings*, **2004**, 858, 283		4
8	Line-broadening and anharmonic effects in the attenuated total reflectance infrared spectra of calcite. *European Journal of Mineralogy*, **2019**, 31, 73-81	2.2	3
7	Electrical characterization of engineered ZnSe?GaAs heterojunction diodes. *Journal of Crystal Growth*, **1997**, 175-176, 603-607	1.6	3
6	Publisher Note: Electron Transport and Hot Phonons in Carbon Nanotubes [Phys. Rev. Lett. 95, 236802 (2005)]. *Physical Review Letters*, **2005**, 95,	7.4	3
5	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	1.3	2
4	Kohn Anomalies and Electron-Phonon Coupling in Carbon Nanotubes. *AIP Conference Proceedings*, **2005**,	0	2
3	Modeling Vibrational EELS: From Bulk to Point Defects. *Microscopy and Microanalysis*, **2020**, 26, 946-947	0.5	1
2	Fermi resonance in the Raman spectrum of graphene. *Physical Review B*, **2020**, 102,	3.3	1
1	First-Principles Modeling of Vibrational Electron Energy Loss Spectra. *Microscopy and Microanalysis*, **2019**, 25, 602-603	0.5	