

# Michele Lazzeri

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Flat Bands and Giant Light-Matter Interaction in Hexagonal Boron Nitride. <i>Physical Review Letters</i> , <b>2021</b> , 127, 137401	7.4	5
116	Single-atom vibrational spectroscopy in the scanning transmission electron microscope. <i>Science</i> , <b>2020</b> , 367, 1124-1127	33.3	73
115	Modeling Vibrational EELS: From Bulk to Point Defects. <i>Microscopy and Microanalysis</i> , <b>2020</b> , 26, 946-947	0.5	1
114	Fermi resonance in the Raman spectrum of graphene. <i>Physical Review B</i> , <b>2020</b> , 102,	3.3	1
113	Structure and stability of silicene on Ag(111) reconstructions from grazing incidence x-ray diffraction and density functional theory. <i>Physical Review B</i> , <b>2019</b> , 99,	3.3	8
112	First-Principles Modeling of Vibrational Electron Energy Loss Spectra. <i>Microscopy and Microanalysis</i> , <b>2019</b> , 25, 602-603	0.5	
111	Line-broadening and anharmonic effects in the attenuated total reflectance infrared spectra of calcite. <i>European Journal of Mineralogy</i> , <b>2019</b> , 31, 73-81	2.2	3
110	Hydrodynamic Heat Transport Regime in Bismuth: A Theoretical Viewpoint. <i>Physical Review Letters</i> , <b>2018</b> , 120, 075901	7.4	15
109	The mechanism for the stabilization and surfactant properties of epitaxial silicene. <i>Nanoscale</i> , <b>2018</b> , 10, 2291-2300	7.7	8
108	Nature of Hexagonal Silicon Forming via High-Pressure Synthesis: Nanostructured Hexagonal 4H Polytype. <i>Nano Letters</i> , <b>2018</b> , 18, 5989-5995	11.5	24
107	New constraints on Xe incorporation mechanisms in olivine from first-principles calculations. <i>Geochimica Et Cosmochimica Acta</i> , <b>2018</b> , 222, 146-155	5.5	12
106	Infrared reflectance, transmittance, and emittance spectra of MgO from first principles. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	6
105	Temperature dependence of X-ray absorption and nuclear magnetic resonance spectra: probing quantum vibrations of light elements in oxides. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 6246-6256	3.6	12
104	Theoretical Raman spectrum and anharmonicity of tetrahedral OH defects in hydrous forsterite. <i>European Journal of Mineralogy</i> , <b>2017</b> , 29, 201-212	2.2	11
103	Infrared spectroscopic study of sulfate-bearing calcite from deep-sea bamboo coral. <i>European Journal of Mineralogy</i> , <b>2017</b> , 29, 397-408	2.2	7
102	Multilayer silicene: clear evidence of Ag-terminated bulk silicon. <i>2D Materials</i> , <b>2017</b> , 4, 025067	5.9	15
101	Advanced capabilities for materials modelling with Quantum ESPRESSO. <i>Journal of Physics Condensed Matter</i> , <b>2017</b> , 29, 465901	1.8	2275

100	First-Principles Vibrational Electron Energy Loss Spectroscopy of Guanine. <i>Physical Review Letters</i> , <b>2017</b> , 119, 027402	7.4	15
99	Nanoscale mechanisms for the reduction of heat transport in bismuth. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	14
98	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. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	20
97	Formation of silicene on silver: Strong interaction between Ag and Si. <i>Physica Status Solidi (B): Basic Research</i> , <b>2016</b> , 253, 206-217	1.3	8
96	Phonon hydrodynamics in two-dimensional materials. <i>Nature Communications</i> , <b>2015</b> , 6, 6400	17.4	282
95	High-field transport in graphene: the impact of Zener tunneling. <i>Journal of Physics Condensed Matter</i> , <b>2015</b> , 27, 164205	1.8	12
94	Reduced partition function ratios of iron and oxygen in goethite. <i>Geochimica Et Cosmochimica Acta</i> , <b>2015</b> , 151, 19-33	5.5	30
93	Growth mechanism of silicene on Ag(111) determined by scanning tunneling microscopy measurements and ab initio calculations. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	31
92	Contribution of interstitial OH groups to the incorporation of water in forsterite. <i>Physics and Chemistry of Minerals</i> , <b>2014</b> , 41, 105-114	1.6	16
91	Thermal conductivity of graphene and graphite: collective excitations and mean free paths. <i>Nano Letters</i> , <b>2014</b> , 14, 6109-14	11.5	353
90	Two-dimensional analysis of the double-resonant 2D Raman mode in bilayer graphene. <i>Physical Review Letters</i> , <b>2014</b> , 113, 187401	7.4	28
89	First-principles modeling of sulfate incorporation and <sup>34</sup> S/ <sup>32</sup> S isotopic fractionation in different calcium carbonates. <i>Chemical Geology</i> , <b>2014</b> , 374-375, 84-91	4.2	19
88	Carbon-Based Nanoscience. <i>Elements</i> , <b>2014</b> , 10, 447-452	3.8	6
87	Theoretical study of the local charge compensation and spectroscopic properties of B-type carbonate defects in apatite. <i>Physics and Chemistry of Minerals</i> , <b>2014</b> , 41, 347-359	1.6	10
86	Infrared spectroscopic properties of goethite: anharmonic broadening, long-range electrostatic effects and Al substitution. <i>Physics and Chemistry of Minerals</i> , <b>2014</b> , 41, 289-302	1.6	19
85	Ab initio variational approach for evaluating lattice thermal conductivity. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	164
84	Raman fingerprint of aligned graphene/h-BN superlattices. <i>Nano Letters</i> , <b>2013</b> , 13, 5242-6	11.5	83
83	Signature of the two-dimensional phonon dispersion in graphene probed by double-resonant Raman scattering. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	50

82	Anharmonic properties from a generalized third-order ab initio approach: Theory and applications to graphite and graphene. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	141
81	Letter. A carbonate-fluoride defect model for carbonate-rich fluorapatite. <i>American Mineralogist</i> , <b>2013</b> , 98, 1066-1069	2.9	53
80	Experimental and theoretical study of the vibrational properties of diaspore ( $\text{AlOOH}$ ). <i>Physics and Chemistry of Minerals</i> , <b>2012</b> , 39, 93-102	1.6	14
79	Hidden polymorphs drive vitrification in $\text{B}_2\text{O}_3$ . <i>Nature Materials</i> , <b>2012</b> , 11, 925-9	27	51
78	Temperature evolution of infrared- and Raman-active phonons in graphite. <i>Physical Review B</i> , <b>2012</b> , 86,	3.3	31
77	First-principles investigation of equilibrium isotopic fractionation of O- and Si-isotopes between refractory solids and gases in the solar nebula. <i>Earth and Planetary Science Letters</i> , <b>2012</b> , 319-320, 118-127	5.3	30
76	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. Saultanov. <i>Geochimica Et Cosmochimica Acta</i> , <b>2012</b> , 87, 356-359	5.5	17
75	First-principles simulation of arsenate adsorption on the (1. <i>Geochimica Et Cosmochimica Acta</i> , <b>2012</b> , 86, 182-195	5.5	35
74	Zener tunneling in the electrical transport of quasimetallic carbon nanotubes. <i>Physical Review B</i> , <b>2012</b> , 86,	3.3	6
73	Variations in the work function of doped single- and few-layer graphene assessed by Kelvin probe force microscopy and density functional theory. <i>Physical Review B</i> , <b>2011</b> , 83,	3.3	152
72	Theory of double-resonant Raman spectra in graphene: Intensity and line shape of defect-induced and two-phonon bands. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	409
71	Line-broadening effects in the powder infrared spectrum of apatite. <i>Physics and Chemistry of Minerals</i> , <b>2011</b> , 38, 111-122	1.6	60
70	Current-voltage characteristics of graphene devices: Interplay between Zener-Klein tunneling and defects. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	67
69	First-principles study of the structural and isotopic properties of Al- and OH-bearing hematite. <i>Geochimica Et Cosmochimica Acta</i> , <b>2010</b> , 74, 3948-3962	5.5	22
68	First-principles calculation of H/D isotopic fractionation between hydrous minerals and water. <i>Geochimica Et Cosmochimica Acta</i> , <b>2010</b> , 74, 3874-3882	5.5	42
67	Clar's theory, pi-electron distribution, and geometry of graphene nanoribbons. <i>Journal of the American Chemical Society</i> , <b>2010</b> , 132, 3440-51	16.4	194
66	Doped graphene as tunable electron-phonon coupling material. <i>Nano Letters</i> , <b>2010</b> , 10, 1172-6	11.5	76
65	Structure and stability of graphene nanoribbons in oxygen, carbon dioxide, water, and ammonia. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	78

64	Pressure-induced phase transitions in amorphous and metastable crystalline germanium by Raman scattering, x-ray spectroscopy, and ab initio calculations. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	35
63	Probing the electrostatic environment of bilayer graphene using Raman spectra. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	36
62	Thermal transport in isotopically disordered carbon nanotubes: a comparison between Green's functions and Boltzmann approaches. <i>Journal of Physics Condensed Matter</i> , <b>2009</b> , 21, 245302	1.8	11
61	The thermodynamic stability and simulated STM images of graphene nanoribbons. <i>Physica Status Solidi (B): Basic Research</i> , <b>2009</b> , 246, 2586-2591	1.3	9
60	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. <i>Journal of Physics Condensed Matter</i> , <b>2009</b> , 21, 395502	1.8	13251
59	Phonon surface mapping of graphite: Disentangling quasi-degenerate phonon dispersions. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	75
58	Theoretical investigation of the anomalous equilibrium fractionation of multiple sulfur isotopes during adsorption. <i>Earth and Planetary Science Letters</i> , <b>2009</b> , 284, 88-93	5.3	20
57	Structural control over equilibrium silicon and oxygen isotopic fractionation: A first-principles density-functional theory study. <i>Chemical Geology</i> , <b>2009</b> , 258, 28-37	4.2	108
56	Iron isotope fractionation between pyrite (FeS <sub>2</sub> ), hematite (Fe <sub>2</sub> O <sub>3</sub> ) and siderite (FeCO <sub>3</sub> ): A first-principles density functional theory study. <i>Geochimica Et Cosmochimica Acta</i> , <b>2009</b> , 73, 6565-6578	5.5	145
55	Boosting electronic transport in carbon nanotubes by isotopic disorder. <i>Physical Review Letters</i> , <b>2009</b> , 102, 196801	7.4	13
54	Ab initio study of gap opening and screening effects in gated bilayer graphene. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	134
53	Transport properties of graphene in the high-current limit. <i>Physical Review Letters</i> , <b>2009</b> , 103, 076601	7.4	177
52	Theoretical infrared absorption coefficient of OH groups in minerals. <i>American Mineralogist</i> , <b>2008</b> , 93, 950-953	2.9	33
51	Boroxol Rings in Liquid and Vitreous B <sub>2</sub> O <sub>3</sub> from First Principles. <i>Physical Review Letters</i> , <b>2008</b> , 101, 065504	7.4	118
50	First-principles calculation of the infrared spectrum of hematite. <i>American Mineralogist</i> , <b>2008</b> , 93, 1019-1027	10.7	32
49	Giant nonadiabatic effects in layer metals: raman spectra of intercalated graphite explained. <i>Physical Review Letters</i> , <b>2008</b> , 100, 226401	7.4	63
48	Surface modes in the infrared spectrum of hydrous minerals: the OH stretching modes of bayerite. <i>Physics and Chemistry of Minerals</i> , <b>2008</b> , 35, 279-285	1.6	46
47	Impact of the electron-electron correlation on phonon dispersion: Failure of LDA and GGA DFT functionals in graphene and graphite. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	237

46	Structure, stability, edge states, and aromaticity of graphene ribbons. <i>Physical Review Letters</i> , <b>2008</b> , 101, 096402	7.4	521
45	Doping in carbon nanotubes probed by Raman and transport measurements. <i>Physical Review Letters</i> , <b>2007</b> , 99, 136803	7.4	123
44	Elasticity of serpentines and extensive serpentinization in subduction zones. <i>Geophysical Research Letters</i> , <b>2007</b> , 34, n/a-n/a	4.9	35
43	Anharmonic and non-adiabatic effects in MgB <sub>2</sub> : Implications for the isotope effect and interpretation of Raman spectra. <i>Physica C: Superconductivity and Its Applications</i> , <b>2007</b> , 456, 38-44	1.3	42
42	Breakdown of the adiabatic approximation in a doped graphene monolayer and in metallic carbon nanotubes. <i>Physica Status Solidi (B): Basic Research</i> , <b>2007</b> , 244, 4118-4123	1.3	2
41	Breakdown of the adiabatic Born-Oppenheimer approximation in graphene. <i>Nature Materials</i> , <b>2007</b> , 6, 198-201	27	1077
40	Structure, reactivity and spectroscopic properties of minerals from lateritic soils: insights from ab initio calculations. <i>European Journal of Soil Science</i> , <b>2007</b> , 58, 870-881	3.4	5
39	Phonon anharmonicities in graphite and graphene. <i>Physical Review Letters</i> , <b>2007</b> , 99, 176802	7.4	327
38	Optical phonons of graphene and nanotubes. <i>European Physical Journal: Special Topics</i> , <b>2007</b> , 148, 159-170	10.5	29
37	Anharmonicity of inner-OH stretching modes in hydrous phyllosilicates: assessment from first-principles frozen-phonon calculations. <i>Physics and Chemistry of Minerals</i> , <b>2007</b> , 34, 621-625	1.6	53
36	Kohn anomalies and nonadiabaticity in doped carbon nanotubes. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	96
35	Equilibrium isotopic fractionation in the kaolinite, quartz, water system: Prediction from first-principles density-functional theory. <i>Geochimica Et Cosmochimica Acta</i> , <b>2007</b> , 71, 3170-3181	5.5	148
34	Optical phonons in carbon nanotubes: Kohn anomalies, Peierls distortions, and dynamic effects. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	393
33	Weak anharmonic effects in MgB <sub>2</sub> : A comparative inelastic x-ray scattering and Raman study. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	35
32	First-principles study of the OH-stretching modes of gibbsite. <i>American Mineralogist</i> , <b>2006</b> , 91, 115-119	2.9	95
31	Raman spectrum of ammonia IV. <i>Physical Review B</i> , <b>2006</b> , 74,	3.3	29
30	Ab initio Raman spectrum of the normal and disordered MgAl <sub>2</sub> O <sub>4</sub> spinel. <i>Physical Review B</i> , <b>2006</b> , 74,	3.3	62
29	Coupled dynamics of electrons and phonons in metallic nanotubes: Current saturation from hot-phonon generation. <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	98

28	Interstitial dinitrogen makes PtN <sub>2</sub> an insulating hard solid. <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	118
27	Surface reconstructions of epitaxial MnAs films grown on GaAs(111)B. <i>Physical Review B</i> , <b>2006</b> , 74,	3.3	15
26	Phonon linewidths and electron-phonon coupling in graphite and nanotubes. <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	290
25	Nonadiabatic Kohn anomaly in a doped graphene monolayer. <i>Physical Review Letters</i> , <b>2006</b> , 97, 266407	7.4	430
24	Raman spectrum of graphene and graphene layers. <i>Physical Review Letters</i> , <b>2006</b> , 97, 187401	7.4	11029
23	First-principles study of OH-stretching modes in kaolinite, dickite, and nacrite. <i>American Mineralogist</i> , <b>2005</b> , 90, 50-60	2.9	58
22	Electron transport and hot phonons in carbon nanotubes. <i>Physical Review Letters</i> , <b>2005</b> , 95, 236802	7.4	224
21	Ab initio resonant Raman spectra of diamond-like carbons. <i>Diamond and Related Materials</i> , <b>2005</b> , 14, 1078-1083	3.5	45
20	Kohn Anomalies and Electron-Phonon Coupling in Carbon Nanotubes. <i>AIP Conference Proceedings</i> , <b>2005</b> ,	0	2
19	Raman spectra of BN nanotubes: Ab initio and bond-polarizability model calculations. <i>Physical Review B</i> , <b>2005</b> , 71,	3.3	36
18	Publisher's Note: Electron Transport and Hot Phonons in Carbon Nanotubes [Phys. Rev. Lett. 95, 236802 (2005)]. <i>Physical Review Letters</i> , <b>2005</b> , 95,	7.4	3
17	Kohn Anomalies in Graphite and Nanotubes. <i>Materials Research Society Symposia Proceedings</i> , <b>2004</b> , 858, 283		4
16	Kohn anomalies and electron-phonon interactions in graphite. <i>Physical Review Letters</i> , <b>2004</b> , 93, 185503	7.4	709
15	Phonon dispersion and lifetimes in MgB <sub>2</sub> . <i>Physical Review Letters</i> , <b>2003</b> , 90, 095506	7.4	126
14	First-principles calculation of vibrational Raman spectra in large systems: signature of small rings in crystalline SiO <sub>2</sub> . <i>Physical Review Letters</i> , <b>2003</b> , 90, 036401	7.4	266
13	Oxygen vacancy mediated adsorption and reactions of molecular oxygen on the TiO <sub>2</sub> (110) surface. <i>Physical Review B</i> , <b>2003</b> , 68,	3.3	99
12	Anharmonic phonon frequency shift in MgB <sub>2</sub> . <i>Physical Review B</i> , <b>2003</b> , 68,	3.3	79
11	High-order density-matrix perturbation theory. <i>Physical Review B</i> , <b>2003</b> , 68,	3.3	16

10	First-principles study of the thermal expansion of Be(101 $\bar{1}0$ ). <i>Physical Review B</i> , <b>2002</b> , 65,	3.3	47
9	Surface oscillatory thermal expansion: Mg(101 $\bar{1}0$ ). <i>Physical Review B</i> , <b>2001</b> , 63,	3.3	10
8	Stress-driven reconstruction of an oxide surface: the anatase TiO <sub>2</sub> (2)(001)-(1 x 4) surface. <i>Physical Review Letters</i> , <b>2001</b> , 87, 266105	7.4	274
7	Structure and energetics of stoichiometric TiO <sub>2</sub> anatase surfaces. <i>Physical Review B</i> , <b>2001</b> , 63,	3.3	1143
6	Ab initio study of Be surface dynamical properties. <i>Surface Science</i> , <b>2000</b> , 454-456, 442-446	1.8	17
5	Ab-initio dynamical properties of the Be(0001) surface. <i>Surface Science</i> , <b>1998</b> , 402-404, 715-718	1.8	26
4	Ab Initio Study of Be (0001) Surface Thermal Expansion. <i>Physical Review Letters</i> , <b>1998</b> , 81, 2096-2099	7.4	44
3	Electrical characterization of engineered ZnSe/GaAs heterojunction diodes. <i>Journal of Crystal Growth</i> , <b>1997</b> , 175-176, 603-607	1.6	3
2	Tuning of ZnSe/GaAs band discontinuities in heterojunction diodes. <i>Applied Physics Letters</i> , <b>1996</b> , 69, 3233-3235	3.4	14
1	Application of Raman spectroscopy to the study of graphitic carbons in the Earth Sciences	415-454	7