Nicola Bonini

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/10069071/publications.pdf

Version: 2024-02-01

33 papers	20,708 citations	393982 19 h-index	433756 31 g-index
33 all docs	33 docs citations	33 times ranked	23844 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	Effect of disorder on Raman scattering of single-layer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mo</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2015, 91, .	1.1	553
3	Role of Disorder and Anharmonicity in the Thermal Conductivity of Silicon-Germanium Alloys: A First-Principles Study. Physical Review Letters, 2011, 106, 045901.	2.9	404
4	Phonon Anharmonicities in Graphite and Graphene. Physical Review Letters, 2007, 99, 176802.	2.9	391
5	Acoustic Phonon Lifetimes and Thermal Transport in Free-Standing and Strained Graphene. Nano Letters, 2012, 12, 2673-2678.	4.5	178
6	Electronâ€“Phonon Interactions and the Intrinsic Electrical Resistivity of Graphene. Nano Letters, 2014, 14, 1113-1119.	4.5	149
7	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
8	High Thermal Conductivity in Short-Period Superlattices. Nano Letters, 2011, 11, 5135-5141.	4.5	81
9	Engineering the Reactivity of Metal Catalysts:Â A Model Study of Methane Dehydrogenation on Rh(111). Journal of the American Chemical Society, 2004, 126, 16732-16733.	6.6	80
10	Thermoelectric coefficients of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>n</mml:mi></mml:math>-doped silicon from first principles via the solution of the Boltzmann transport equation. Physical Review B, 2016, 94, .	1.1	71
11	Methane Dehydrogenation on Rh@Cu(111):Â A First-Principles Study of a Model Catalyst. Journal of the American Chemical Society, 2006, 128, 12448-12454.	6.6	60
12	Theory-Guided Synthesis of an Eco-Friendly and Low-Cost Copper Based Sulfide Thermoelectric Material. Journal of Physical Chemistry C, 2016, 120, 27135-27140.	1.5	60
13	Enhanced thermoelectric performance of Sn-doped Cu₃SbS₄. Journal of Materials Chemistry C, 2018, 6, 8546-8552.	2.7	59
14	First-principles predictions of Hall and drift mobilities in semiconductors. Physical Review Research, 2021, 3, .	1.3	48
15	Bulk aluminum at high pressure: A first-principles study. Physical Review B, 2008, 77, .	1.1	42
16	Dominant phonon wave vectors and strain-induced splitting of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>2</mml:mn><mml:mi>D</mml:mi></mml:mrow></mml:math>Raman mode of graphene. Physical Review B, 2012, 85, .	1.1	34
17	Magnetotransport phenomena in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>p</mml:mi></mml:math> -doped diamond from first principles. Physical Review B, 2018, 98, .	1.1	31
18	Spin-Flop Ordering from Frustrated Ferro- and Antiferromagnetic Interactions: A Combined Theoretical and Experimental Study of aMn/Fe(100)Monolayer. Physical Review Letters, 2005, 95, 117201.	2.9	27

#	Article	IF	Citations
19	Lattice anharmonicity in lowâ€dimensional carbon systems. Physica Status Solidi (B): Basic Research, 2008, 245, 2149-2154.	0.7	25
20	Laurdan and Di-4-ANEPPDHQ Influence the Properties of Lipid Membranes: A Classical Molecular Dynamics and Fluorescence Study. Journal of Physical Chemistry B, 2020, 124, 11419-11430.	1.2	20
21	Subsurface Oxygen Stabilization by a Third Species:â€‰ Carbonates on Ag(210). Journal of Physical Chemistry C, 2007, 111, 10923-10930.	1.5	16
22	Structural and electronic evolution in the Cu₃SbS₄â€“Cu₃SnS₄solid solution. Journal of Materials Chemistry C, 2020, 8, 11508-11516.	2.7	16
23	Theory and Computation of Hall Scattering Factor in Graphene. Nano Letters, 2020, 20, 8861-8865.	4.5	13
24	On-surface and sub-surface oxygen adsorption on Ag(210): Vibrational properties. Surface Science, 2005, 587, 50-54.	0.8	12
25	First-principles study of electronic transport and structural properties of Cu12Sb4S13 in its high-temperature phase. Physical Review Research, 2020, 2, .	1.3	10
26	Dominant phonon wavevectors of the 2D Raman mode of graphene. Physica Status Solidi (B): Basic Research, 2011, 248, 2635-2638.	0.7	9
27	First-Principles Determination of Phonon Lifetimes, Mean Free Paths, and Thermal Conductivities in Crystalline Materials: Pure Silicon and Germanium. Topics in Applied Physics, 2014, , 115-136.	0.4	9
28	Thermomechanical properties of honeycomb lattices from internal-coordinates potentials: the case of graphene and hexagonal boron nitride. 2D Materials, 2021, 8, 015026.	2.0	7
29	Customising excitation properties of polycyclic aromatic hydrocarbons by rational positional heteroatom doping: the peri-xanthenoxanthene (PXX) case. Chemical Science, 0, , .	3.7	5
30	Structural Evolution in BiNbO4. Inorganic Chemistry, 2021, 60, 8507-8518.	1.9	4
31	High-Temperature Superconductivity in the Lanthanide Hydrides at Extreme Pressures. Applied Sciences (Switzerland), 2022, 12, 874.	1.3	4
32	Computational materials discovery for lanthanide hydrides at high pressure for high temperature superconductivity. Physical Review Research, 2022, 4, .	1.3	2
33	Exploring the Effect of the Number of Hydrogen Atoms on the Properties of Lanthanide Hydrides by DMFT. Applied Sciences (Switzerland), 2022, 12, 3498.	1.3	0