Andrea Floris

List of Publications by Year
in descending order

48 papers	7,058 citations	218677 26 h-index	223800 46 g-index
49 all docs	49 docs citations	49 times ranked	8893 citing authors

#	Article	IF	Citations
1	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	1.8	4,303
2	Hubbard-corrected DFT energy functionals: The LDA+U description of correlated systems. International Journal of Quantum Chemistry, 2014, 114, 14-49.	2.0	533
3	Ab initiotheory of superconductivity. I. Density functional formalism and approximate functionals. Physical Review B, 2005, 72, .	3.2	314
4	Ab initiotheory of superconductivity. II. Application to elemental metals. Physical Review B, 2005, 72, .	3.2	261
5	AbÂInitioDescription of High-Temperature Superconductivity in Dense Molecular Hydrogen. Physical Review Letters, 2008, 100, 257001.	7.8	199
6	Superconductivity in Lithium, Potassium, and Aluminum under Extreme Pressure: A First-Principles Study. Physical Review Letters, 2006, 96, 047003.	7.8	159
7	Superconducting Properties ofMgB2from First Principles. Physical Review Letters, 2005, 94, 037004.	7.8	137
8	Anisotropic gap of superconductingCaC6: A first-principles density functional calculation. Physical Review B, 2007, 75, .	3.2	101
9	Stereoselectivity and electrostatics in charge-transfer Mn- and Cs-TCNQ4 networks on Ag(100). Nature Communications, 2012, 3, 940.	12.8	90
10	Vibrational properties of MnO and NiO from DFT<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mo>+</mml:mo><mml:mspace width="0.28em" /><mml:mi>U</mml:mi></mml:mrow></mml:math>-based density functional perturbation theory. Physical Review B, 2011, 84, .	3.2	82
11	Two-band superconductivity in Pb fromab initiocalculations. Physical Review B, 2007, 75, .	3.2	73
12	Exact Conditions in Finite-Temperature Density-Functional Theory. Physical Review Letters, 2011, 107, 163001.	7.8	73
13	Electron-phonon interaction and superconductivity in metallic molecular hydrogen. II. Superconductivity under pressure. Physical Review B, 2010, 81, .	3.2	60
14	Thermoelasticity of Fe²⁺â€bearing bridgmanite. Geophysical Research Letters, 2015, 42, 1741-1749.	4.0	57
15	Thermostatic properties of nitrate molten salts and their solar and eutectic mixtures. Scientific Reports, 2018, 8, 10485.	3.3	48
16	Electron-phonon interaction and superconductivity in metallic molecular hydrogen. I. Electronic and dynamical properties under pressure. Physical Review B, 2010, 81, .	3.2	47
17	Superconducting properties of MgB2 from first principles. Physica C: Superconductivity and Its Applications, 2007, 456, 45-53.	1.2	46
18	Hubbard-corrected density functional perturbation theory with ultrasoft pseudopotentials. Physical Review B, 2020, 101, .	3.2	43

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19	Ab initioprediction of pressure-induced superconductivity in potassium. Physical Review B, 2006, 73, .	3.2	41
20	Reduced partition function ratios of iron and oxygen in goethite. Geochimica Et Cosmochimica Acta, 2015, 151, 19-33.	3.9	38
21	Electronic, vibrational, and superconducting properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mtext>CaBeSi</mml:mtext></mml:mrow></mml:mrow></mml:math>: First-principles calculations. Physical Review B, 2009, 79, .	3.2	32
22	The role of Coulomb interaction in the superconducting properties of CaC₆and H under pressure. Superconductor Science and Technology, 2009, 22, 034006.	3.5	32
23	Driving Forces for Covalent Assembly of Porphyrins by Selective Câ€“H Bond Activation and Intermolecular Coupling on a Copper Surface. Journal of the American Chemical Society, 2016, 138, 5837-5847.	13.7	30
24	Anomalous Coarsening Driven by Reversible Charge Transfer at Metalâ€“Organic Interfaces. ACS Nano, 2014, 8, 12356-12364.	14.6	27
25	First-Principles Calculation of the Real-Space Order Parameter and Condensation Energy Density in Phonon-Mediated Superconductors. Physical Review Letters, 2015, 115, 097002.	7.8	26
26	A Small Molecule Walks Along a Surface Between Porphyrin Fences That Are Assembled Inâ€…Situ. Angewandte Chemie - International Edition, 2015, 54, 7101-7105.	13.8	26
27	Infrared spectroscopic properties of goethite: anharmonic broadening, long-range electrostatic effects and Al substitution. Physics and Chemistry of Minerals, 2014, 41, 289-302.	0.8	24
28	Fast Molecular Compression by a Hyperthermal Collision Gives Bond-Selective Mechanochemistry. Physical Review Letters, 2021, 126, 056001.	7.8	22
29	AbÂInitio Electron-Phonon Interactions in Correlated Electron Systems. Physical Review Letters, 2021, 127, 126404.	7.8	22
30	Fine-Tuning the Electrostatic Properties of an Alkali-Linked Organic Adlayer on a Metal Substrate. ACS Nano, 2013, 7, 8059-8065.	14.6	21
31	Probing the electron-phonon coupling in MgB 2 through magnetoresistance measurements in neutron irradiated thin films. Europhysics Letters, 2008, 81, 67006.	2.0	12
32	Multiband superconductivity in Pb, H under pressure and CaBeSi fromab initiocalculations. Journal of Physics Condensed Matter, 2009, 21, 164209.	1.8	10
33	Mechanisms of Covalent Dimerization on a Bulk Insulating Surface. Journal of Physical Chemistry C, 2017, 121, 10053-10062.	3.1	9
34	A Small Molecule Walks Along a Surface Between Porphyrin Fences That Are Assembled Inâ€…Situ. Angewandte Chemie, 2015, 127, 7207-7211.	2.0	7
35	Increasing the Templating Effect on a Bulk Insulator Surface: From a Kinetically Trapped to a Thermodynamically More Stable Structure. Journal of Physical Chemistry C, 2016, 120, 17546-17554.	3.1	7
36	On-surface synthesis on a bulk insulator surface. Journal of Physics Condensed Matter, 2018, 30, 133001.	1.8	7

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37	Kinetic control of molecular assembly on surfaces. Communications Chemistry, 2018, 1, .	4.5	6
38	Controlling the preferential motion of chiral molecular walkers on a surface. Chemical Science, 2019, 10, 5864-5874.	7.4	6
39	Unified Description of the Specific Heat of Ionic Bulk Materials Containing Nanoparticles. ACS Nano, 2021, 15, 563-574.	14.6	6
40	Cu doping effects inMgB2. Physical Review B, 2003, 67, .	3.2	5
41	Publisherâ€™s Note:Ab initioDescription of High-Temperature Superconductivity in Dense Molecular Hydrogen [Phys. Rev. Lett.100, 257001 (2008)]. Physical Review Letters, 2008, 101, .	7.8	4
42	Creating a regular array of metal-complexing molecules on an insulator surface at room temperature. Nature Communications, 2020, 11, 6424.	12.8	3
43	Magnetic Energy Landscape of Dimolybdenum Tetraacetate on a Bulk Insulator Surface. Applied Sciences (Switzerland), 2021, 11, 3806.	2.5	3
44	Ab-initio Computation of Superconducting Properties of Elemental Superconductors and MgB2. Journal of Superconductivity and Novel Magnetism, 2005, 18, 649-652.	0.5	2
45	Ethylene Dissociation on Ni₃Al(111). Journal of Physical Chemistry C, 2017, 121, 7967-7976.	3.1	2
46	Focus on the Essential: Extracting the Decisive Energy Barrier of a Complex Process. Advanced Materials Interfaces, 2019, 6, 1900795.	3.7	2
47	Energy Barrier: Focus on the Essential: Extracting the Decisive Energy Barrier of a Complex Process (Adv. Mater. Interfaces 20/2019). Advanced Materials Interfaces, 2019, 6, 1970128.	3.7	0
48	Special issue on novel superconducting and magnetic materials. Journal of Physics Condensed Matter, 2020, 32, 040401.	1.8	0