Matteo Cococcioni

List of Publications by Year
in descending order

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25 papers	23,500 citations	394421 19 h-index	552781 26 g-index
27 all docs	27 docs citations	27 times ranked	24745 citing authors

#	Article	IF	Citations
1	Energy Level Alignment at the Cobalt Phosphate/Electrolyte Interface: Intrinsic Stability vs Interfacial Chemical Reactions in 5 V Lithium Ion Batteries. ACS Applied Materials & Interfaces, 2022, 14, 543-556.	8.0	4
2	HP â€“ A code for the calculation of Hubbard parameters using density-functional perturbation theory. Computer Physics Communications, 2022, 279, 108455.	7.5	35
3	Self-consistent Hubbard parameters from density-functional perturbation theory in the ultrasoft and projector-augmented wave formulations. Physical Review B, 2021, 103, .	3.2	84
4	Magnetic Energy Landscape of Dimolybdenum Tetraacetate on a Bulk Insulator Surface. Applied Sciences (Switzerland), 2021, 11, 3806.	2.5	3
5	The Different Story of Ï€ Bonds. Molecules, 2021, 26, 3805.	3.8	2
6	AbÂInitio Electron-Phonon Interactions in Correlated Electron Systems. Physical Review Letters, 2021, 127, 126404.	7.8	22
7	Optimizing accuracy and efficacy in data-driven materials discovery for the solar production of hydrogen. Energy and Environmental Science, 2021, 14, 2335-2348.	30.8	23
8	Pulay forces in density-functional theory with extended Hubbard functionals: From nonorthogonalized to orthogonalized manifolds. Physical Review B, 2020, 102, .	3.2	22
9	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>LDA</mml:mi><mml:mo>+</mml:mo><mml:msub><mml:mi calculations of phase relations in FeO. Physical Review Materials, 2020, 4, .	2.4	14
10	Electronic structure of pristine and Ni-substituted <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>La</mml:mi><mml:mi>Fe</mml:mi><mml:msub><mml:m mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> from near edge x-ray absorption fine structure experiments and first-principles simulations. Physical	3.6	17
11	Energetics and cathode voltages of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Li</mml:mi><mml:mi>M</mml:mi><mml:msub><mml:mi olivines (<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 337 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML"><m	3.6	38
12	Hubbard parameters from density-functional perturbation theory. Physical Review B, 2018, 98, .	3.2	194
13	DFT calculation and experimental investigation of Mn doping effect in Fe16N2. AIP Advances, 2016, 6, .	1.3	20
14	Atomic bonding effects in annular dark field scanning transmission electron microscopy. I. Computational predictions. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2016, 34, .	2.1	3
15	Hubbard-corrected DFT energy functionals: The LDA+U description of correlated systems. International Journal of Quantum Chemistry, 2014, 114, 14-49.	2.0	533
16	Bridging density-functional and many-body perturbation theory: Orbital-density dependence in electronic-structure functionals. Physical Review B, 2014, 89, .	3.2	32
17	Î²-Scission of Olefins on Acidic Zeolites: A Periodic PBE-D Study in H-ZSM-5. Journal of Physical Chemistry C, 2013, 117, 23609-23620.	3.1	58
18	First principles calculation of the electronic properties and lattice dynamics of Cu2ZnSn(S1â˜xSex)4. Journal of Applied Physics, 2012, 111, .	2.5	73

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19	Density Functional Theory Study on the Adsorption of H₂S and Other Claus Process Tail Gas Components on Copper- and Silver-Exchanged Y Zeolites. Journal of Physical Chemistry C, 2012, 116, 3561-3575.	3.1	37
20	Calculation of the lattice dynamics and Raman spectra of copper zinc tin chalcogenides and comparison to experiments. Journal of Applied Physics, 2012, 111, .	2.5	221
21	Koopmansâ€™ condition for density-functional theory. Physical Review B, 2010, 82, .	3.2	206
22	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502.	1.8	18,183
23	Density Functional Theory in Transition-Metal Chemistry: A Self-Consistent HubbardUApproach. Physical Review Letters, 2006, 97, 103001.	7.8	526
24	Linear response approach to the calculation of the effective interaction parameters in theLDA+Umethod. Physical Review B, 2005, 71, .	3.2	2,754
25	The Li intercalation potential of LiMPO4 and LiMSiO4 olivines with M=Fe, Mn, Co, Ni. Electrochemistry Communications, 2004, 6, 1144-1148.	4.7	390