Kurt Lejaeghere

List of Publications by Year
in descending order

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23 papers	3,241 citations	430874 18 h-index	677142 22 g-index
23 all docs	23 docs citations	23 times ranked	5846 citing authors

#	Article	IF	Citations
1	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
2	Thermal unequilibrium of strained black CsPbI ₃ thin films. Science, 2019, 365, 679-684.	12.6	444
3	Error Estimates for Solid-State Density-Functional Theory Predictions: An Overview by Means of the Ground-State Elemental Crystals. Critical Reviews in Solid State and Materials Sciences, 2014, 39, 1-24.	12.3	404
4	The Abinitproject: Impact, environment and recent developments. Computer Physics Communications, 2020, 248, 107042.	7.5	369
5	Missing Linkers: An Alternative Pathway to UiO-66 Electronic Structure Engineering. Chemistry of Materials, 2017, 29, 3006-3019.	6.7	176
6	Understanding Intrinsic Light Absorption Properties of UiO-66 Frameworks: A Combined Theoretical and Experimental Study. Inorganic Chemistry, 2015, 54, 10701-10710.	4.0	155
7	First-Principles Study of Antisite Defect Configurations in ZnGa₂O₄:Cr Persistent Phosphors. Inorganic Chemistry, 2016, 55, 2402-2412.	4.0	106
8	Error estimates for density-functional theory predictions of surface energy and work function. Physical Review B, 2016, 94, .	3.2	96
9	Tuning the balance between dispersion and entropy to design temperature-responsive flexible metal-organic frameworks. Nature Communications, 2018, 9, 4899.	12.8	90
10	Exploring Lanthanide Doping in UiO-66: A Combined Experimental and Computational Study of the Electronic Structure. Inorganic Chemistry, 2018, 57, 5463-5474.	4.0	51
11	Mechanical Properties from Periodic Plane Wave Quantum Mechanical Codes: The Challenge of the Flexible Nanoporous MIL-47(V) Framework. Journal of Physical Chemistry C, 2015, 119, 23752-23766.	3.1	37
12	Precision of Electric-Field Gradient Predictions by Density Functional Theory and Implications for the Nuclear Quadrupole Moment and Its Error Bar of the 111Cd 245 keV 5/2+ Level. Journal of Physical Chemistry C, 2016, 120, 23111-23120.	3.1	27
13	Assessment of a low-cost protocol for anab initiobased prediction of the mixing enthalpy at elevated temperatures: The Fe-Mo system. Physical Review B, 2011, 83, .	3.2	23
14	Ranking the Stars: A Refined Pareto Approach to Computational Materials Design. Physical Review Letters, 2013, 111, 075501.	7.8	23
15	Quasi-1D physics in metal-organic frameworks: MIL-47(V) from first principles. Beilstein Journal of Nanotechnology, 2014, 5, 1738-1748.	2.8	23
16	Ab initiobased thermal property predictions at a low cost: An error analysis. Physical Review B, 2014, 89, .	3.2	23
17	Charge transfer induced energy storage in CaZnOS:Mn â€“ insight from experimental and computational spectroscopy. Physical Chemistry Chemical Physics, 2017, 19, 9075-9085.	2.8	21
18	Carbon capture turned upside down: high-temperature adsorption & low-temperature desorption (HALD). Energy and Environmental Science, 2015, 8, 2480-2491.	30.8	19

#	Article	IF	Citations
19	Is the error on first-principles volume predictions absolute or relative?. Computational Materials Science, 2016, 117, 390-396.	3.0	15
20	A first-principles reassessment of the Fe-N phase diagram in the low-nitrogen limit. Journal of Alloys and Compounds, 2019, 775, 758-768.	5.5	9
21	Optical Properties of Isolated and Covalent Organic Framework-Embedded Ruthenium Complexes. Journal of Physical Chemistry A, 2019, 123, 6854-6867.	2.5	7
22	Electronic properties of heterogenized Ru(<scp>ii</scp>) polypyridyl photoredox complexes on covalent triazine frameworks. Journal of Materials Chemistry A, 2019, 7, 8433-8442.	10.3	6
23	The uncertainty pyramid for electronic-structure methods. , 2020, , 41-76.		4