Sebastian Schwalbe

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4579102/publications.pdf

Version: 2024-02-01

17	276	1040056 9	888059 17
papers	citations	h-index	g-index

22	22	22	265
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	porE : A code for deterministic and systematic analyses of porosities. Journal of Computational Chemistry, 2021, 42, 630-643.	3.3	4
2	Chemical bonding theories as guides for self-interaction corrected solutions: Multiple local minima and symmetry breaking. Journal of Chemical Physics, 2021, 155, 224109.	3.0	7
3	PyFLOSIC: Python-based Fermiâ€“LÃ¶wdin orbital self-interaction correction. Journal of Chemical Physics, 2020, 153, 084104.	3.0	17
4	Interpretation and Automatic Generation of Fermiâ€Orbital Descriptors. Journal of Computational Chemistry, 2019, 40, 2843-2857.	3.3	21
5	Stretched or noded orbital densities and self-interaction correction in density functional theory. Journal of Chemical Physics, 2019, 150, 174102.	3.0	46
6	Analytic atomic gradients in the fermiâ€Ã¶wdin orbital selfâ€interaction correction. Journal of Computational Chemistry, 2019, 40, 820-825.	3.3	16
7	Fermiâ€LÃ¶wdin orbital selfâ€interaction corrected density functional theory: Ionization potentials and enthalpies of formation. Journal of Computational Chemistry, 2018, 39, 2463-2471.	3.3	35
8	Theoretical and experimental investigations of ¹²⁹Xe NMR chemical shift isotherms in metalâ€“organic frameworks. Physical Chemistry Chemical Physics, 2018, 20, 25039-25043.	2.8	8
9	Ni^{II}formate complexes with bi- and tridentate nitrogen-donor ligands: synthesis, characterization, and magnetic and thermal properties. Dalton Transactions, 2017, 46, 3963-3979.	3.3	8
10	Mechanical, elastic and thermodynamic properties of crystalline lithium silicides. Computational Materials Science, 2017, 134, 48-57.	3.0	4
11	The origin of the measured chemical shift of ¹²⁹Xe in UiO-66 and UiO-67 revealed by DFT investigations. Physical Chemistry Chemical Physics, 2017, 19, 10020-10027.	2.8	23
12	Symmetry Breaking within Fermiâ€“LÃ¶wdin Orbital Self-Interaction Corrected Density Functional Theory. Journal of Chemical Theory and Computation, 2017, 13, 5823-5828.	5.3	6
13	Thermodynamic characterization of lithium monosilicide (LiSi) by means of calorimetry and DFT-calculations. International Journal of Materials Research, 2017, 108, 942-958.	0.3	8
14	Ab initioelectronic structure and optical conductivity of bismuth tellurohalides. Physical Review B, 2016, 94, .	3.2	18
15	Screening for high-spin metal organic frameworks (MOFs): density functional theory study on DUT-8(M₁,M₂) (with M_i = V,â€¦,Cu). Physical Chemistry Chemical Physics, 2016, 18, 8075-8080.	2.8	23
16	Electronic and magnetic properties of DUT-8(Ni). Physical Chemistry Chemical Physics, 2015, 17, 17122-17129.	2.8	29
17	Testing Selfâ€interaction Correction for Molecules in Solution. Advanced Engineering Materials, 0, , 2100572.	3.5	1