James W Furness

List of Publications by Year
in descending order

14	777	759233 12	996975 15
papers	citations	h-index	g-index

17	17	17	499
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Accurate and Numerically Efficient r²SCAN Meta-Generalized Gradient Approximation. Journal of Physical Chemistry Letters, 2020, 11, 8208-8215.	4.6	335
2	An accurate first-principles treatment of doping-dependent electronic structure of high-temperature cuprate superconductors. Communications Physics, 2018, 1, .	5.3	94
3	r2SCAN-D4: Dispersion corrected meta-generalized gradient approximation for general chemical applications. Journal of Chemical Physics, 2021, 154, 061101.	3.0	70
4	Symmetry-breaking polymorphous descriptions for correlated materials without interelectronic U. Physical Review B, 2020, 102, .	3.2	48
5	Enhancing the efficiency of density functionals with an improved iso-orbital indicator. Physical Review B, 2019, 99, .	3.2	37
6	Subtlety of TiO2 phase stability: Reliability of the density functional theory predictions and persistence of the self-interaction error. Journal of Chemical Physics, 2019, 150, 014105.	3.0	32
7	Construction of meta-GGA functionals through restoration of exact constraint adherence to regularized SCAN functionals. Journal of Chemical Physics, 2022, 156, 034109.	3.0	25
8	First-principles calculation of spin and orbital contributions to magnetically ordered moments in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sr</mml:mi><mml:mn>2</mml:mn></mml:r Physical Review B, 2020, 101, .	3.2	23
9	Self-Consistent Field Methods for Excited States in Strong Magnetic Fields: a Comparison between Energy- and Variance-Based Approaches. Journal of Chemical Theory and Computation, 2021, 17, 5492-5508.	5.3	16
10	Tunable catalytic activity of cobalt-intercalated layered MnO2 for water oxidation through confinement and local ordering. Journal of Catalysis, 2019, 374, 143-149.	6.2	13
11	Sensitivity of the electronic and magnetic structures of cuprate superconductors to density functional approximations. Npj Computational Materials, 2022, 8, .	8.7	12
12	Reliable Lattice Dynamics from an Efficient Density Functional Approximation. Chemistry of Materials, 2022, 34, 2562-2568.	6.7	12
13	Examining the order-of-limits problem and lattice constant performance of the Taoâ€“Mo functional. Journal of Chemical Physics, 2020, 152, 244112.	3.0	11
14	Connections between variation principles at the interface of wave-function and density-functional theories. Journal of Chemical Physics, 2017, 147, 134107.	3.0	4