Zeng-hui Yang

List of Publications by Year
in descending order

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25 papers	2,147 citations	623188 14 h-index	580395 25 g-index
29 all docs	29 docs citations	29 times ranked	2873 citing authors

#	Article	IF	Citations
1	Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. Nature Chemistry, 2016, 8, 831-836.	6.6	698
2	Understanding band gaps of solids in generalized Kohnâ€“Sham theory. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2801-2806.	3.3	423
3	Versatile van der Waals Density Functional Based on a Meta-Generalized Gradient Approximation. Physical Review X, 2016, 6, .	2.8	321
4	More realistic band gaps from meta-generalized gradient approximations: Only in a generalized Kohn-Sham scheme. Physical Review B, 2016, 93, .	1.1	182
5	A Brief Compendium of Time-Dependent Density Functional Theory. Brazilian Journal of Physics, 2014, 44, 154-188.	0.7	84
6	Full self-consistency in the Fermi-orbital self-interaction correction. Physical Review A, 2017, 95, .	1.0	76
7	Simple screened exact-exchange approach for excitonic properties in solids. Physical Review B, 2015, 92, .	1.1	55
8	Exact and approximate Kohn-Sham potentials in ensemble density-functional theory. Physical Review A, 2014, 90, .	1.0	48
9	Direct calculation of exciton binding energies with time-dependent density-functional theory. Physical Review B, 2013, 87, .	1.1	44
10	Excitations and benchmark ensemble density functional theory for two electrons. Journal of Chemical Physics, 2014, 140, 18A541.	1.2	42
11	Direct Extraction of Excitation Energies from Ensemble Density-Functional Theory. Physical Review Letters, 2017, 119, 033003.	2.9	38
12	A minimal model for excitons within time-dependent density-functional theory. Journal of Chemical Physics, 2012, 137, 014513.	1.2	26
13	Excitons in Time-Dependent Density-Functional Theory. Topics in Current Chemistry, 2014, 368, 185-217.	4.0	20
14	Communication: Near-locality of exchange and correlation density functionals for 1- and 2-electron systems. Journal of Chemical Physics, 2016, 144, 191101.	1.2	20
15	Effect of Cusps in Time-Dependent Quantum Mechanics. Physical Review Letters, 2012, 108, 063003.	2.9	13
16	First-principles study of the binding energy between nanostructures and its scaling with system size. Physical Review B, 2018, 97, .	1.1	13
17	Nonexistence of a Taylor expansion in time due to cusps. Physical Review A, 2013, 88, .	1.0	7
18	Extending scaled-interaction adaptive-partitioning QM/MM to covalently bonded systems. Physical Chemistry Chemical Physics, 2020, 22, 17987-17998.	1.3	7

#	Article	IF	Citations
19	Must Kohnâ€“Sham oscillator strengths be accurate at threshold?. Journal of Chemical Physics, 2009, 131, 114308.	1.2	6
20	Displacement damage in silicon studied by the electronic force field method in the keV regime. Computational Materials Science, 2020, 179, 109697.	1.4	6
21	Gamma-ray irradiation-induced oxidation and disproportionation at the amorphous SiO₂/Si interfaces. Journal of Materials Chemistry C, 2020, 8, 17065-17073.	2.7	5
22	Speed-dependent adaptive partitioning in QM/MM MD simulations of displacement damage in solid-state systems. Physical Chemistry Chemical Physics, 2021, 23, 3417-3428.	1.3	4
23	Enhancing magnetic dipole emission in Eu-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Sr</mml:mi><mml:mi>M</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> () Tj ETQq1 1 0.784314 rgBT /Ov	1.1	4
24	On-the-fly determination of active region centers in adaptive-partitioning QM/MM. Physical Chemistry Chemical Physics, 2020, 22, 19307-19317.	1.3	3
25	Second-order perturbative correlation energy functional in the ensemble density-functional theory. Physical Review A, 2021, 104, .	1.0	2