

Zeng-hui Yang

List of Publications by Year in descending order

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Version: 2024-02-01

25
papers

2,147
citations

623574

14
h-index

580701

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

#	ARTICLE	IF	CITATIONS
19	Must Kohn "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 SiO ₂ /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 SrM_2O_7 (Tj ETQq1 1,0,784314,rgBT /Ove	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