

# Zeng-hui Yang

## List of Publications by Year in descending order

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Version: 2024-02-01

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	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
2	Enhancing magnetic dipole emission in Eu-doped $\text{SrMgSiO}_3$ by surface modification. Journal of Materials Chemistry C, 2020, 8, 17065-17073.	1.1	4
3	Second-order perturbative correlation energy functional in the ensemble density-functional theory. Physical Review A, 2021, 104, .	1.0	2
4	Gamma-ray irradiation-induced oxidation and disproportionation at the amorphous $\text{SiO}_2/\text{Si}$ interfaces. Journal of Materials Chemistry C, 2020, 8, 17065-17073.	2.7	5
5	Extending scaled-interaction adaptive-partitioning QM/MM to covalently bonded systems. Physical Chemistry Chemical Physics, 2020, 22, 17987-17998.	1.3	7
6	On-the-fly determination of active region centers in adaptive-partitioning QM/MM. Physical Chemistry Chemical Physics, 2020, 22, 19307-19317.	1.3	3
7	Displacement damage in silicon studied by the electronic force field method in the keV regime. Computational Materials Science, 2020, 179, 109697.	1.4	6
8	First-principles study of the binding energy between nanostructures and its scaling with system size. Physical Review B, 2018, 97, .	1.1	13
9	Understanding band gaps of solids in generalized Kohn-Sham theory. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2801-2806.	3.3	423
10	Direct Extraction of Excitation Energies from Ensemble Density-Functional Theory. Physical Review Letters, 2017, 119, 033003.	2.9	38
11	Full self-consistency in the Fermi-orbital self-interaction correction. Physical Review A, 2017, 95, .	1.0	76
12	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
13	More realistic band gaps from meta-generalized gradient approximations: Only in a generalized Kohn-Sham scheme. Physical Review B, 2016, 93, .	1.1	182
14	Versatile van der Waals Density Functional Based on a Meta-Generalized Gradient Approximation. Physical Review X, 2016, 6, .	2.8	321
15	Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. Nature Chemistry, 2016, 8, 831-836.	6.6	698
16	Simple screened exact-exchange approach for excitonic properties in solids. Physical Review B, 2015, 92, .	1.1	55
17	Exact and approximate Kohn-Sham potentials in ensemble density-functional theory. Physical Review A, 2014, 90, .	1.0	48
18	Excitons in Time-Dependent Density-Functional Theory. Topics in Current Chemistry, 2014, 368, 185-217.	4.0	20

#	ARTICLE	IF	CITATIONS
19	A Brief Compendium of Time-Dependent Density Functional Theory. Brazilian Journal of Physics, 2014, 44, 154-188.	0.7	84
20	Excitations and benchmark ensemble density functional theory for two electrons. Journal of Chemical Physics, 2014, 140, 18A541.	1.2	42
21	Direct calculation of exciton binding energies with time-dependent density-functional theory. Physical Review B, 2013, 87, .	1.1	44
22	Nonexistence of a Taylor expansion in time due to cusps. Physical Review A, 2013, 88, .	1.0	7
23	Effect of Cusps in Time-Dependent Quantum Mechanics. Physical Review Letters, 2012, 108, 063003.	2.9	13
24	A minimal model for excitons within time-dependent density-functional theory. Journal of Chemical Physics, 2012, 137, 014513.	1.2	26
25	Must Kohn-Sham oscillator strengths be accurate at threshold?. Journal of Chemical Physics, 2009, 131, 114308.	1.2	6