Yi Yao

List of Publications by Year
in descending order

19	564	623734	794594
papers	citations	14	19
		h-index	g-index

20	20	20	567
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	All-Electron BSE@GW Method for K-Edge Core Electron Excitation Energies. Journal of Chemical Theory and Computation, 2022, 18, 1569-1583.	5.3	20
2	All-electron periodic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:m implementation with numerical atomic orbital basis functions: Algorithm and benchmarks. Physical Review Materials, 2021, 5, .	2.4	25
3	Charge transfer states and carrier generation in 1D organolead iodide semiconductors. Journal of Materials Chemistry A, 2021, 9, 14977-14990.	10.3	15
4	Nuclear Quantum Effect and Its Temperature Dependence in Liquid Water from Random Phase Approximation via Artificial Neural Network. Journal of Physical Chemistry Letters, 2021, 12, 6354-6362.	4.6	16
5	Simulating electronic excitation and dynamics with real-time propagation approach to TDDFT within plane-wave pseudopotential formulation. Journal of Chemical Physics, 2021, 155, 100901.	3.0	24
6	All-electron real-time and imaginary-time time-dependent density functional theory within a numeric atom-centered basis function framework. Journal of Chemical Physics, 2021, 155, 154801.	3.0	14
7	First-Principles Modeling of Electronic Stopping in Complex Matter under Ion Irradiation. Journal of Physical Chemistry Letters, 2020, 11, 229-237.	4.6	13
8	Temperature dependence of nuclear quantum effects on liquid water via artificial neural network model based on SCAN meta-GGA functional. Journal of Chemical Physics, 2020, 153, 044114.	3.0	22
9	All-electron ab initio Bethe-Salpeter equation approach to neutral excitations in molecules with numeric atom-centered orbitals. Journal of Chemical Physics, 2020, 152, 044105.	3.0	38
10	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>K</mml:mi></mml:mrow></mml:math> -Shell Core-Electron Excitations in Electronic Stopping of Protons in Water from First Principles. Physical Review Letters, 2019, 123, 066401.	7.8	34
11	Propagation of maximally localized Wannier functions in real-time TDDFT. Journal of Chemical Physics, 2019, 150, 194113.	3.0	20
12	Free Energy Profile of NaCl in Water: First-Principles Molecular Dynamics with SCAN and Ï‰B97X-V Exchangeâ€“Correlation Functionals. Journal of Chemical Theory and Computation, 2018, 14, 884-893.	5.3	41
13	Examining real-time time-dependent density functional theory nonequilibrium simulations for the calculation of electronic stopping power. Physical Review B, 2017, 96, .	3.2	60
14	Plane-wave pseudopotential implementation and performance of SCAN meta-GGA exchange-correlation functional for extended systems. Journal of Chemical Physics, 2017, 146, 224105.	3.0	66
15	Diffusion quantum Monte Carlo study of martensitic phase transition energetics: The case of phosphorene. Journal of Chemical Physics, 2016, 145, 124705.	3.0	7
16	Electronic stopping power in liquid water for protons and Î± particles from first principles. Physical Review B, 2016, 94, .	3.2	46
17	Communication: Modeling of concentration dependent water diffusivity in ionic solutions: Role of intermolecular charge transfer. Journal of Chemical Physics, 2015, 143, 241101.	3.0	53
18	Reptation Quantum Monte Carlo calculation of charge transfer: The Naâ€“Cl dimer. Chemical Physics Letters, 2015, 618, 236-240.	2.6	4

#	Article	IF	Citations
19	Role of Charge Transfer in Water Diffusivity in Aqueous Ionic Solutions. Journal of Physical Chemistry Letters, 2014, 5, 2711-2716.	4.6	46