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	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
2	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
3	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
4	Role of Charge Transfer in Water Diffusivity in Aqueous Ionic Solutions. Journal of Physical Chemistry Letters, 2014, 5, 2711-2716.	4.6	46
5	Electronic stopping power in liquid water for protons and Î± particles from first principles. Physical Review B, 2016, 94, .	3.2	46
6	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
7	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
8	<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
9	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:msub></mml:mrow></mml:math> implementation with numerical atomic orbital basis functions: Algorithm and benchmarks. Physical Review Materials, 2021, 5, .	2.4	25
10	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
11	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
12	Propagation of maximally localized Wannier functions in real-time TDDFT. Journal of Chemical Physics, 2019, 150, 194113.	3.0	20
13	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
14	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
15	Charge transfer states and carrier generation in 1D organolead iodide semiconductors. Journal of Materials Chemistry A, 2021, 9, 14977-14990.	10.3	15
16	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
17	First-Principles Modeling of Electronic Stopping in Complex Matter under Ion Irradiation. Journal of Physical Chemistry Letters, 2020, 11, 229-237.	4.6	13
18	Diffusion quantum Monte Carlo study of martensitic phase transition energetics: The case of phosphorene. Journal of Chemical Physics, 2016, 145, 124705.	3.0	7

#	Article	IF	Citations
19	Reptation Quantum Monte Carlo calculation of charge transfer: The Naâ€“Cl dimer. Chemical Physics Letters, 2015, 618, 236-240.	2.6	4