Feizhi Ding

List of Publications by Year in descending order

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36 papers	2,001 citations	236925 25 h-index	345221 36 g-index
37 all docs	37 docs citations	37 times ranked	3249 citing authors

#	Article	IF	Citations
1	Small Nuclear Quantum Effects in Scattering of H and D from Graphene. Journal of Physical Chemistry Letters, 2021, 12, 1991-1996.	4.6	17
2	The Chronus Quantum software package. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1436.	14.6	66
3	Embedded Mean-Field Theory for Solution-Phase Transition-Metal Polyolefin Catalysis. Journal of Chemical Theory and Computation, 2020, 16, 4226-4237.	5.3	3
4	Analytical gradients for projection-based wavefunction-in-DFT embedding. Journal of Chemical Physics, 2019, 151, .	3.0	17
5	Imaging covalent bond formation by H atom scattering from graphene. Science, 2019, 364, 379-382.	12.6	76
6	Achieving high-performance thick-film perovskite solar cells with electron transporting Bingel fullerenes. Journal of Materials Chemistry A, 2018, 6, 15495-15503.	10.3	32
7	Modulate Molecular Interaction between Hole Extraction Polymers and Lead Ions toward Hysteresisâ€Free and Efficient Perovskite Solar Cells. Advanced Materials Interfaces, 2018, 5, 1800090.	3.7	18
8	Molecular Engineered Holeâ€Extraction Materials to Enable Dopantâ€Free, Efficient pâ€iâ€n Perovskite Solar Cells. Advanced Energy Materials, 2017, 7, 1700012.	19.5	195
9	Embedded Mean-Field Theory with Block-Orthogonalized Partitioning. Journal of Chemical Theory and Computation, 2017, 13, 1605-1615.	5.3	35
10	Doping Versatile n-Type Organic Semiconductors via Room Temperature Solution-Processable Anionic Dopants. ACS Applied Materials & Interfaces, 2017, 9, 1136-1144.	8.0	35
11	Linear-Response Time-Dependent Embedded Mean-Field Theory. Journal of Chemical Theory and Computation, 2017, 13, 4216-4227.	5.3	20
12	Highly Sensitive Builtâ€In Strain Sensors for Polymer Composites: Fluorescence Turnâ€On Response through Mechanochemical Activation. Advanced Materials, 2016, 28, 6592-6597.	21.0	56
13	Aromatic thiol-mediated cleavage of Nâ€“O bonds enables chemical ubiquitylation of folded proteins. Nature Communications, 2016, 7, 12979.	12.8	52
14	Approximate singly excited states from a two-component Hartree-Fock reference. Journal of Chemical Physics, 2015, 143, 144106.	3.0	10
15	Ab initio two-component Ehrenfest dynamics. Journal of Chemical Physics, 2015, 143, 114105.	3.0	31
16	Enhanced Performance of Organic Solar Cells with Increased End Group Dipole Moment in Indacenodithieno[3,2â€b]thiopheneâ€Based Molecules. Advanced Functional Materials, 2015, 25, 4889-4897.	14.9	61
17	Stability of the complex generalized Hartree-Fock equations. Journal of Chemical Physics, 2015, 142, 154109.	3.0	29
18	Real-Time TDDFT Studies of Exciton Decay and Transfer in Silver Nanowire Arrays. Journal of Physical Chemistry C, 2015, 119, 6421-6427.	3.1	46

#	Article	IF	Citations
19	A conductive liquid crystal via facile doping of an n-type benzodifurandione derivative. Journal of Materials Chemistry A, 2015, 3, 6929-6934.	10.3	14
20	Time-dependent non-equilibrium dielectric response in QM/continuum approaches. Journal of Chemical Physics, 2015, 142, 034120.	3.0	31
21	Quantum coherent plasmon in silver nanowires: A real-time TDDFT study. Journal of Chemical Physics, 2014, 140, 244705.	3.0	57
22	Ab initio non-relativistic spin dynamics. Journal of Chemical Physics, 2014, 141, 214111.	3.0	20
23	Density of States Guided MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Chemical Theory and Computation, 2014, 10, 1910-1914.	5.3	2
24	A Guided Self-Consistent-Field Method for Excited-State Wave Function Optimization: Applications to Ligand-Field Transitions in Transition-Metal Complexes. Journal of Chemical Theory and Computation, 2013, 9, 3933-3938.	5.3	24
25	An efficient method for calculating dynamical hyperpolarizabilities using real-time time-dependent density functional theory. Journal of Chemical Physics, 2013, 138, 064104.	3.0	72
26	Doping of Fullerenes via Anionâ€Induced Electron Transfer and Its Implication for Surfactant Facilitated High Performance Polymer Solar Cells. Advanced Materials, 2013, 25, 4425-4430.	21.0	244
27	Solutionâ€Processible Highly Conducting Fullerenes. Advanced Materials, 2013, 25, 2457-2461.	21.0	130
28	Solvated First-Principles Excited-State Charge-Transfer Dynamics with Time-Dependent Polarizable Continuum Model and Solvent Dielectric Relaxation. Journal of Physical Chemistry Letters, 2012, 3, 2898-2904.	4.6	40
29	Mechanisms of bridge-mediated electron transfer: A TDDFT electronic dynamics study. Journal of Chemical Physics, 2012, 137, 22A512.	3.0	22
30	On the gauge invariance of nonperturbative electronic dynamics using the time-dependent Hartree-Fock and time-dependent Kohn-Sham. Journal of Chemical Physics, 2011, 135, 164101.	3.0	41
31	Computational Study of Bridge-Assisted Intervalence Electron Transfer. Journal of Physical Chemistry A, 2010, 114, 6039-6046.	2.5	50
32	Computational Study of Ferrocene-Based Molecular Frameworks with 2,5-Diethynylpyridine as a Chemical Bridge. Materials, 2010, 3, 2668-2683.	2.9	37
33	First-Principles Calculation of pK_aValues for Organic Acids in Nonaqueous Solution. Journal of Organic Chemistry, 2009, 74, 2679-2691.	3.2	129
34	Ligand Dependence of Binding to Three-Coordinate Fe(II) Complexes. Inorganic Chemistry, 2009, 48, 5106-5116.	4.0	35
35	Nanoparticle-Mediated Intervalence Transfer. Journal of the American Chemical Society, 2008, 130, 12156-12162.	13.7	59
36	Thermodynamics of Hydrogen Atom Transfer to a High-Valent Iron Imido Complex. Journal of the American Chemical Society, 2008, 130, 2716-2717.	13.7	188