Xinguo Ren

List of Publications by Year in Descending Order

59 papers	4,638 citations	26 h-index	64 g-index
64 ext. papers	5,347 ext. citations	4.1 avg, IF	5.4 L-index

#	Paper	IF	Citations
59	Real-Time, Time-Dependent Density Functional Theory Study on Photoinduced Isomerizations of Azobenzene Under a Light Field.. *Journal of Physical Chemistry Letters*, **2022**, 427-432	6.4	2
58	Phase stability of the argon crystal: first-principles study based on random phase approximation plus renormalized single excitation corrections. *New Journal of Physics*, **2022**, 24, 033049	2.9	1
57	Beryllium and Magnesium Metal Clusters: New Globally Stable Structures and Calculations. *Journal of Physical Chemistry A*, **2021**, 125, 1424-1435	2.8	3
56	Self-Interaction-Corrected Random Phase Approximation. *Journal of Chemical Theory and Computation*, **2021**, 17, 2107-2115	6.4	1
55	Real-time -BSE investigations on spin-valley exciton dynamics in monolayer transition metal dichalcogenide. *Science Advances*, **2021**, 7,	14.3	23
54	First-principles study of benzo[a]pyrene-7,8-dione and DNA adducts. *Journal of Chemical Physics*, **2021**, 154, 175102	3.9	0
53	Retention and recycling of deuterium in liquid lithium-tin slab studied by first-principles molecular dynamics. *Journal of Nuclear Materials*, **2021**, 543, 152542	3.3	1
52	Efficient Hybrid Density Functional Calculations for Large Periodic Systems Using Numerical Atomic Orbitals. *Journal of Chemical Theory and Computation*, **2021**, 17, 222-239	6.4	1
51	All-electron periodic G0W0 implementation with numerical atomic orbital basis functions: Algorithm and benchmarks. *Physical Review Materials*, **2021**, 5,	3.2	11
50	Assessing the Approach: Beyond with Hedin's Full Second-Order Self-Energy Contribution. *Journal of Chemical Theory and Computation*, **2021**, 17, 5140-5154	6.4	3
49	Accurate stress calculations based on numerical atomic orbital bases: Implementation and benchmarks. *Computer Physics Communications*, **2021**, 267, 108043	4.2	
48	Accuracy of Localized Resolution of the Identity in Periodic Hybrid Functional Calculations with Numerical Atomic Orbitals. *Journal of Physical Chemistry Letters*, **2020**, 11, 3082-3088	6.4	6
47	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	3.9	22
46	Intercalation of van der Waals layered materials: A route towards engineering of electron correlation. *Chinese Physics B*, **2020**, 29, 097104	1.2	3
45	First-principles calculation of optical responses based on nonorthogonal localized orbitals. *New Journal of Physics*, **2019**, 21, 093001	2.9	1
44	Comparing particle-particle and particle-hole channels of the random phase approximation. *Physical Review B*, **2019**, 99,	3.3	2
43	Identifying Different Adsorption States of Methanol on ZnO(101 0): A Scanning Tunneling Microscopy and Density Functional Theory Study. *Journal of Physical Chemistry C*, **2019**, 123, 9105-9111	3.8	5

42	Main-group test set for materials science and engineering with user-friendly graphical tools for error analysis: systematic benchmark of the numerical and intrinsic errors in state-of-the-art electronic-structure approximations. *New Journal of Physics*, **2019**, 21, 013025	2.9	10
41	Cooperative Effect in a Graphite Intercalation Compound: Enhanced Mobility of AlCl4 in the Graphite Cathode of Aluminum-Ion Batteries. *Physical Review Applied*, **2019**, 12,	4.3	4
40	A DFT study of energetic and structural properties of a full turn of A-form DNA under relaxed and stretching conditions. *Journal of Chemical Physics*, **2019**, 151, 215102	3.9	5
39	First-principles study of the electronic and optical properties of Li(Nb,Os)O3 alloys. *Applied Physics Letters*, **2018**, 112, 103901	3.4	4
38	First-principles calculations and model analysis of plasmon excitations in graphene and graphene/hBN heterostructure. *Physical Review B*, **2017**, 96,	3.3	8
37	First-principles molecular dynamics study of deuterium diffusion in liquid tin. *Journal of Chemical Physics*, **2017**, 147, 064505	3.9	6
36	Density functional theory study of the Þphase transition in cerium: Role of electron correlation and f-orbital localization. *Physical Review B*, **2016**, 93,	3.3	15
35	Enforcing the linear behavior of the total energy with hybrid functionals: Implications for charge transfer, interaction energies, and the random-phase approximation. *Physical Review B*, **2016**, 94,	3.3	40
34	Self-consistent Green¥ function embedding for advanced electronic structure methods based on a dynamical mean-field concept. *Physical Review B*, **2016**, 93,	3.3	26
33	Strong charge and spin fluctuations in La2O3Fe2Se2. *Physical Review B*, **2016**, 94,	3.3	4
32	Large-scale ab initio simulations based on systematically improvable atomic basis. *Computational Materials Science*, **2016**, 112, 503-517	3.2	31
31	Metal adatoms generated by the co-play of melamine assembly and subsequent CO adsorption. *Physical Chemistry Chemical Physics*, **2016**, 18, 2324-9	3.6	7
30	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules III: A Benchmark of GW Methods. *Journal of Chemical Theory and Computation*, **2016**, 12, 615-26	6.4	119
29	The origin of hyperferroelectricity in LiBO (B = V, Nb, Ta, Os). *Scientific Reports*, **2016**, 6, 34085	4.9	14
28	Exploring Molecules beyond CO as Tip Functionalizations in High-Resolution Noncontact Atomic Force Microscopy: A First Principles Approach. *ACS Omega*, **2016**, 1, 1004-1009	3.9	4
27	Directional Growth of One-Dimensional CO2 Chains on ZnO(101 0). *Journal of Physical Chemistry C*, **2016**, 120, 23669-23674	3.8	12
26	Hybrid functionals for large periodic systems in an all-electron, numeric atom-centered basis framework. *Computer Physics Communications*, **2015**, 192, 60-69	4.2	89
25	GW100: Benchmarking G0W0 for Molecular Systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 5665-87	6.4	207

24	Accurate localized resolution of identity approach for linear-scaling hybrid density functionals and for many-body perturbation theory. *New Journal of Physics*, **2015**, 17, 093020	2.9	65
23	Beyond the GW approximation: A second-order screened exchange correction. *Physical Review B*, **2015**, 92,	3.3	37
22	Static correlation and electron localization in molecular dimers from the self-consistent RPA and GW approximation. *Physical Review B*, **2015**, 91,	3.3	46
21	Origin of the Contrast Interpreted as Intermolecular and Intramolecular Bonds in Atomic Force Microscopy Images. *Journal of Physical Chemistry C*, **2015**, 119, 14195-14200	3.8	26
20	High-Resolution Model for Noncontact Atomic Force Microscopy with a Flexible Molecule on the Tip Apex. *Journal of Physical Chemistry C*, **2015**, 119, 1483-1488	3.8	29
19	First-principles description of charge transfer in donor-acceptor compounds from self-consistent many-body perturbation theory. *Physical Review B*, **2014**, 90,	3.3	42
18	Size Effects in the Interface Level Alignment of Dye-Sensitized TiO2 Clusters. *Journal of Physical Chemistry Letters*, **2014**, 5, 2395-401	6.4	24
17	On the room-temperature phase diagram of high pressure hydrogen: an ab initio molecular dynamics perspective and a diffusion Monte Carlo study. *Journal of Chemical Physics*, **2014**, 141, 024501	3.9	18
16	Self-consistent GW: All-electron implementation with localized basis functions. *Physical Review B*, **2013**, 88,	3.3	120
15	Bond breaking and bond formation: how electron correlation is captured in many-body perturbation theory and density-functional theory. *Physical Review Letters*, **2013**, 110, 146403	7.4	69
14	Structure and energetics of benzene adsorbed on transition-metal surfaces: density-functional theory with van der Waals interactions including collective substrate response. *New Journal of Physics*, **2013**, 15, 053046	2.9	129
13	Numeric atom-centered-orbital basis sets with valence-correlation consistency from H to Ar. *New Journal of Physics*, **2013**, 15, 123033	2.9	65
12	Renormalized second-order perturbation theory for the electron correlation energy: Concept, implementation, and benchmarks. *Physical Review B*, **2013**, 88,	3.3	88
11	Random-phase approximation and its applications in computational chemistry and materials science. *Journal of Materials Science*, **2012**, 47, 7447-7471	4.3	389
10	Toward Low-Temperature Dehydrogenation Catalysis: Isophorone Adsorbed on Pd(111). *Journal of Physical Chemistry Letters*, **2012**, 3, 582-6	6.4	33
9	Benchmark of GW methods for azabenzenes. *Physical Review B*, **2012**, 86,	3.3	132
8	Resolution-of-identity approach to Hartree–Fock, hybrid density functionals, RPA, MP2 and GW with numeric atom-centered orbital basis functions. *New Journal of Physics*, **2012**, 14, 053020	2.9	411
7	Assessment of correlation energies based on the random-phase approximation. *New Journal of Physics*, **2012**, 14, 043002	2.9	111

6	Density-functional theory for f-electron systems: the □phase transition in cerium. *Physical Review Letters*, **2012**, 109, 146402	7.4	51
5	Beyond the random-phase approximation for the electron correlation energy: the importance of single excitations. *Physical Review Letters*, **2011**, 106, 153003	7.4	171
4	Electronic structure of dye-sensitized TiO2 clusters from many-body perturbation theory. *Physical Review B*, **2011**, 84,	3.3	38
3	Electronic structure of copper phthalocyanine from G0W0 calculations. *Physical Review B*, **2011**, 84,	3.3	80
2	Exploring the random phase approximation: Application to CO adsorbed on Cu(111). *Physical Review B*, **2009**, 80,	3.3	136
1	Ab initio molecular simulations with numeric atom-centered orbitals. *Computer Physics Communications*, **2009**, 180, 2175-2196	4.2	1637