

# Xinguo Ren

## List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Ab initio molecular simulations with numeric atom-centered orbitals. <i>Computer Physics Communications</i> , <b>2009</b> , 180, 2175-2196	4.2	1637
58	Resolution-of-identity approach to Hartree-Fock, hybrid density functionals, RPA, MP2 and GW with numeric atom-centered orbital basis functions. <i>New Journal of Physics</i> , <b>2012</b> , 14, 053020	2.9	411
57	Random-phase approximation and its applications in computational chemistry and materials science. <i>Journal of Materials Science</i> , <b>2012</b> , 47, 7447-7471	4.3	389
56	GW100: Benchmarking G0W0 for Molecular Systems. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 5665-87	6.4	207
55	Beyond the random-phase approximation for the electron correlation energy: the importance of single excitations. <i>Physical Review Letters</i> , <b>2011</b> , 106, 153003	7.4	171
54	Exploring the random phase approximation: Application to CO adsorbed on Cu(111). <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	136
53	Benchmark of GW methods for azabenzenes. <i>Physical Review B</i> , <b>2012</b> , 86,	3.3	132
52	Structure and energetics of benzene adsorbed on transition-metal surfaces: density-functional theory with van der Waals interactions including collective substrate response. <i>New Journal of Physics</i> , <b>2013</b> , 15, 053046	2.9	129
51	Self-consistent GW: All-electron implementation with localized basis functions. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	120
50	Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules III: A Benchmark of GW Methods. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 615-26	6.4	119
49	Assessment of correlation energies based on the random-phase approximation. <i>New Journal of Physics</i> , <b>2012</b> , 14, 043002	2.9	111
48	Hybrid functionals for large periodic systems in an all-electron, numeric atom-centered basis framework. <i>Computer Physics Communications</i> , <b>2015</b> , 192, 60-69	4.2	89
47	Renormalized second-order perturbation theory for the electron correlation energy: Concept, implementation, and benchmarks. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	88
46	Electronic structure of copper phthalocyanine from G0W0 calculations. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	80
45	Bond breaking and bond formation: how electron correlation is captured in many-body perturbation theory and density-functional theory. <i>Physical Review Letters</i> , <b>2013</b> , 110, 146403	7.4	69
44	Accurate localized resolution of identity approach for linear-scaling hybrid density functionals and for many-body perturbation theory. <i>New Journal of Physics</i> , <b>2015</b> , 17, 093020	2.9	65
43	Numeric atom-centered-orbital basis sets with valence-correlation consistency from H to Ar. <i>New Journal of Physics</i> , <b>2013</b> , 15, 123033	2.9	65

42	Density-functional theory for f-electron systems: the $\mathbb{H}$ phase transition in cerium. <i>Physical Review Letters</i> , <b>2012</b> , 109, 146402	7.4	51
41	Static correlation and electron localization in molecular dimers from the self-consistent RPA and GW approximation. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	46
40	First-principles description of charge transfer in donor-acceptor compounds from self-consistent many-body perturbation theory. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	42
39	Enforcing the linear behavior of the total energy with hybrid functionals: Implications for charge transfer, interaction energies, and the random-phase approximation. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	40
38	Electronic structure of dye-sensitized TiO <sub>2</sub> clusters from many-body perturbation theory. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	38
37	Beyond the GW approximation: A second-order screened exchange correction. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	37
36	Toward Low-Temperature Dehydrogenation Catalysis: Isophorone Adsorbed on Pd(111). <i>Journal of Physical Chemistry Letters</i> , <b>2012</b> , 3, 582-6	6.4	33
35	Large-scale ab initio simulations based on systematically improvable atomic basis. <i>Computational Materials Science</i> , <b>2016</b> , 112, 503-517	3.2	31
34	High-Resolution Model for Noncontact Atomic Force Microscopy with a Flexible Molecule on the Tip Apex. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 1483-1488	3.8	29
33	Self-consistent Green's function embedding for advanced electronic structure methods based on a dynamical mean-field concept. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	26
32	Origin of the Contrast Interpreted as Intermolecular and Intramolecular Bonds in Atomic Force Microscopy Images. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 14195-14200	3.8	26
31	Size Effects in the Interface Level Alignment of Dye-Sensitized TiO <sub>2</sub> Clusters. <i>Journal of Physical Chemistry Letters</i> , <b>2014</b> , 5, 2395-401	6.4	24
30	Real-time -BSE investigations on spin-valley exciton dynamics in monolayer transition metal dichalcogenide. <i>Science Advances</i> , <b>2021</b> , 7,	14.3	23
29	All-electron ab initio Bethe-Salpeter equation approach to neutral excitations in molecules with numeric atom-centered orbitals. <i>Journal of Chemical Physics</i> , <b>2020</b> , 152, 044105	3.9	22
28	On the room-temperature phase diagram of high pressure hydrogen: an ab initio molecular dynamics perspective and a diffusion Monte Carlo study. <i>Journal of Chemical Physics</i> , <b>2014</b> , 141, 024501	3.9	18
27	Density functional theory study of the $\mathbb{H}$ phase transition in cerium: Role of electron correlation and f-orbital localization. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	15
26	The origin of hyperferroelectricity in LiBO (B = V, Nb, Ta, Os). <i>Scientific Reports</i> , <b>2016</b> , 6, 34085	4.9	14
25	Directional Growth of One-Dimensional CO <sub>2</sub> Chains on ZnO(101 0). <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 23669-23674	3.8	12

24	All-electron periodic G0W0 implementation with numerical atomic orbital basis functions: Algorithm and benchmarks. <i>Physical Review Materials</i> , <b>2021</b> , 5,	3.2	11
23	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. <i>New Journal of Physics</i> , <b>2019</b> , 21, 013025	2.9	10
22	First-principles calculations and model analysis of plasmon excitations in graphene and graphene/hBN heterostructure. <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	8
21	Metal adatoms generated by the co-play of melamine assembly and subsequent CO adsorption. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 2324-9	3.6	7
20	Accuracy of Localized Resolution of the Identity in Periodic Hybrid Functional Calculations with Numerical Atomic Orbitals. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 3082-3088	6.4	6
19	First-principles molecular dynamics study of deuterium diffusion in liquid tin. <i>Journal of Chemical Physics</i> , <b>2017</b> , 147, 064505	3.9	6
18	Identifying Different Adsorption States of Methanol on ZnO(101 0): A Scanning Tunneling Microscopy and Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 9105-9111	3.8	5
17	A DFT study of energetic and structural properties of a full turn of A-form DNA under relaxed and stretching conditions. <i>Journal of Chemical Physics</i> , <b>2019</b> , 151, 215102	3.9	5
16	First-principles study of the electronic and optical properties of Li(Nb,Os)O <sub>3</sub> alloys. <i>Applied Physics Letters</i> , <b>2018</b> , 112, 103901	3.4	4
15	Strong charge and spin fluctuations in La <sub>2</sub> O <sub>3</sub> Fe <sub>2</sub> Se <sub>2</sub> . <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	4
14	Cooperative Effect in a Graphite Intercalation Compound: Enhanced Mobility of AlCl <sub>4</sub> in the Graphite Cathode of Aluminum-Ion Batteries. <i>Physical Review Applied</i> , <b>2019</b> , 12,	4.3	4
13	Exploring Molecules beyond CO as Tip Functionalizations in High-Resolution Noncontact Atomic Force Microscopy: A First Principles Approach. <i>ACS Omega</i> , <b>2016</b> , 1, 1004-1009	3.9	4
12	Beryllium and Magnesium Metal Clusters: New Globally Stable Structures and Calculations. <i>Journal of Physical Chemistry A</i> , <b>2021</b> , 125, 1424-1435	2.8	3
11	Intercalation of van der Waals layered materials: A route towards engineering of electron correlation. <i>Chinese Physics B</i> , <b>2020</b> , 29, 097104	1.2	3
10	Assessing the $\Gamma$ Approach: Beyond with Hedin's Full Second-Order Self-Energy Contribution. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 5140-5154	6.4	3
9	Comparing particle-particle and particle-hole channels of the random phase approximation. <i>Physical Review B</i> , <b>2019</b> , 99,	3.3	2
8	Real-Time, Time-Dependent Density Functional Theory Study on Photoinduced Isomerizations of Azobenzene Under a Light Field.. <i>Journal of Physical Chemistry Letters</i> , <b>2022</b> , 427-432	6.4	2
7	First-principles calculation of optical responses based on nonorthogonal localized orbitals. <i>New Journal of Physics</i> , <b>2019</b> , 21, 093001	2.9	1

6	Self-Interaction-Corrected Random Phase Approximation. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 2107-2115	6.4	1
5	Retention and recycling of deuterium in liquid lithium-tin slab studied by first-principles molecular dynamics. <i>Journal of Nuclear Materials</i> , <b>2021</b> , 543, 152542	3.3	1
4	Efficient Hybrid Density Functional Calculations for Large Periodic Systems Using Numerical Atomic Orbitals. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 222-239	6.4	1
3	Phase stability of the argon crystal: first-principles study based on random phase approximation plus renormalized single excitation corrections. <i>New Journal of Physics</i> , <b>2022</b> , 24, 033049	2.9	1
2	First-principles study of benzo[a]pyrene-7,8-dione and DNA adducts. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 175102	3.9	0
1	Accurate stress calculations based on numerical atomic orbital bases: Implementation and benchmarks. <i>Computer Physics Communications</i> , <b>2021</b> , 267, 108043	4.2	