Jianwei Sun

List of Publications by Citations

77 papers	6,358 citations	33 h-index	79 g-index
89 ext. papers	7,900 ext. citations	6.3 avg, IF	6.37 L-index

#	Paper	IF	Citations
77	Strongly Constrained and Appropriately Normed Semilocal Density Functional. *Physical Review Letters*, **2015**, 115, 036402	7.4	1431
76	Density functional theory is straying from the path toward the exact functional. *Science*, **2017**, 355, 49-52	33.3	548
75	Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. *Nature Chemistry*, **2016**, 8, 831-6	17.6	480
74	Workhorse semilocal density functional for condensed matter physics and quantum chemistry. *Physical Review Letters*, **2009**, 103, 026403	7.4	426
73	Understanding band gaps of solids in generalized Kohn-Sham theory. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 2801-2806	11.5	280
72	Some Fundamental Issues in Ground-State Density Functional Theory: A Guide for the Perplexed. *Journal of Chemical Theory and Computation*, **2009**, 5, 902-8	6.4	273
71	Versatile van der Waals Density Functional Based on a Meta-Generalized Gradient Approximation. *Physical Review X*, **2016**, 6,	9.1	213
70	Energetics of MnO2 polymorphs in density functional theory. *Physical Review B*, **2016**, 93,	3.3	147
69	Density functionals that recognize covalent, metallic, and weak bonds. *Physical Review Letters*, **2013**, 111, 106401	7.4	143
68	Self-consistent meta-generalized gradient approximation within the projector-augmented-wave method. *Physical Review B*, **2011**, 84,	3.3	138
67	Semilocal and hybrid meta-generalized gradient approximations based on the understanding of the kinetic-energy-density dependence. *Journal of Chemical Physics*, **2013**, 138, 044113	3.9	136
66	More realistic band gaps from meta-generalized gradient approximations: Only in a generalized Kohn-Sham scheme. *Physical Review B*, **2016**, 93,	3.3	135
65	Efficient first-principles prediction of solid stability: Towards chemical accuracy. *Npj Computational Materials*, **2018**, 4,	10.9	107
64	Properties of real metallic surfaces: Effects of density functional semilocality and van der Waals nonlocality. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E9188-E9196	11.5	105
63	Communication: Effect of the orbital-overlap dependence in the meta generalized gradient approximation. *Journal of Chemical Physics*, **2012**, 137, 051101	3.9	102
62	Semilocal density functional obeying a strongly tightened bound for exchange. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 685-9	11.5	101
61	Comparative first-principles studies of prototypical ferroelectric materials by LDA, GGA, and SCAN meta-GGA. *Physical Review B*, **2017**, 96,	3.3	96

60	Accurate and Numerically Efficient rSCAN Meta-Generalized Gradient Approximation. *Journal of Physical Chemistry Letters*, **2020**, 11, 8208-8215	6.4	87
59	Accurate critical pressures for structural phase transitions of group IV, III-V, and II-VI compounds from the SCAN density functional. *Physical Review B*, **2018**, 97,	3.3	74
58	Testing density functionals for structural phase transitions of solids under pressure: Si, SiO2, and Zr. *Physical Review B*, **2013**, 88,	3.3	74
57	van der Waals bilayer energetics: Generalized stacking-fault energy of graphene, boron nitride, and graphene/boron nitride bilayers. *Physical Review B*, **2015**, 92,	3.3	74
56	Performance of meta-GGA Functionals on General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. *Journal of Chemical Theory and Computation*, **2013**, 9, 355-63	6.4	62
55	Improved lattice constants, surface energies, and CO desorption energies from a semilocal density functional. *Physical Review B*, **2011**, 83,	3.3	59
54	Gedanken densities and exact constraints in density functional theory. *Journal of Chemical Physics*, **2014**, 140, 18A533	3.9	56
53	Semilocal density functionals and constraint satisfaction. *International Journal of Quantum Chemistry*, **2016**, 116, 847-851	2.1	56
52	Copper-Intercalated Birnessite as a Water Oxidation Catalyst. *Langmuir*, **2015**, 31, 12807-13	4	55
51	An accurate first-principles treatment of doping-dependent electronic structure of high-temperature cuprate superconductors. *Communications Physics*, **2018**, 1,	5.4	55
50	Lattice constants from semilocal density functionals with zero-point phonon correction. *Physical Review B*, **2012**, 85,	3.3	52
49	Antiferromagnetic ground state of La2CuO4: A parameter-free ab initio description. *Physical Review B*, **2018**, 98,	3.3	45
48	A meta-GGA Made Free of the Order of Limits Anomaly. *Journal of Chemical Theory and Computation*, **2012**, 8, 2078-87	6.4	44
47	Correlation energy of the uniform electron gas from an interpolation between high- and low-density limits. *Physical Review B*, **2010**, 81,	3.3	43
46	First-Principles Prediction of a Stable Hexagonal Phase of CH3NH3PbI3. *Chemistry of Materials*, **2017**, 29, 6003-6011	9.6	40
45	Response to Comment on "Density functional theory is straying from the path toward the exact functional". *Science*, **2017**, 356, 496	33.3	38
44	Competing stripe and magnetic phases in the cuprates from first principles. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 68-72	11.5	33
43	Water Oxidation Catalyzed by Cobalt Oxide Supported on the Mattagamite Phase of CoTe2. *ACS Catalysis*, **2016**, 6, 7393-7397	13.1	32

42	Accuracy of first-principles interatomic interactions and predictions of ferroelectric phase transitions in perovskite oxides: Energy functional and effective Hamiltonian. *Physical Review B*, **2017**, 95,	3.3	31
41	Rethinking CO adsorption on transition-metal surfaces: Effect of density-driven self-interaction errors. *Physical Review B*, **2019**, 100,	3.3	29
40	Adsorption and Deposition of Li2O2 on TiC{111} Surface. *Journal of Physical Chemistry Letters*, **2014** , 5, 3919-23	6.4	28
39	Enhancing the efficiency of density functionals with an improved iso-orbital indicator. *Physical Review B*, **2019**, 99,	3.3	26
38	Structural phase transitions in Si and SiO2 crystals via the random phase approximation. *Physical Review B*, **2012**, 86,	3.3	24
37	Accurate, precise, and efficient theoretical methods to calculate anion-□interaction energies in model structures. *Journal of Chemical Theory and Computation*, **2015**, 11, 360-71	6.4	23
36	Dependence of the structure and dynamics of liquid silicon on the choice of density functional approximation. *Physical Review B*, **2017**, 96,	3.3	22
35	Combinations of coupled cluster, density functionals, and the random phase approximation for describing static and dynamic correlation, and van der Waals interactions. *Molecular Physics*, **2016**, 114, 997-1018	1.7	22
34	rSCAN-D4: Dispersion corrected meta-generalized gradient approximation for general chemical applications. *Journal of Chemical Physics*, **2021**, 154, 061101	3.9	22
33	Symmetry-breaking polymorphous descriptions for correlated materials without interelectronic U. *Physical Review B*, **2020**, 102,	3.3	19
32	Subtlety of TiO phase stability: Reliability of the density functional theory predictions and persistence of the self-interaction error. *Journal of Chemical Physics*, **2019**, 150, 014105	3.9	19
31	Interpretations of ground-state symmetry breaking and strong correlation in wavefunction and density functional theories. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	18
30	Why Density Functionals Should Not Be Judged Primarily by Atomization Energies. *Periodica Polytechnica: Chemical Engineering*, **2016**, 60, 2-7	1.3	17
29	Magnetic and f-electron effects in LaNiO2 and NdNiO2 nickelates with cuprate-like (3{d}_{{x}^{2}-{y}^{2}}) band. *Communications Physics*, **2021**, 4,	5.4	16
28	Coulomb correlation in noncollinear antiferromagnetic □Mn. *Physical Review B*, **2020**, 101,	3.3	15
27	van der Waals interaction as a summable asymptotic series. *Physical Review A*, **2012**, 86,	2.6	15
26	Intensive Atomization Energy: Re-Thinking a Metric for Electronic Structure Theory Methods. *Zeitschrift Fur Physikalische Chemie*, **2016**, 230, 737-742	3.1	14
25	Communication: Near-locality of exchange and correlation density functionals for 1- and 2-electron systems. *Journal of Chemical Physics*, **2016**, 144, 191101	3.9	14

24	First-principles calculation of spin and orbital contributions to magnetically ordered moments in Sr2IrO4. *Physical Review B*, **2020**, 101,	3.3	12
23	Spinon excitations in the quasi-one-dimensional S=12 chain compound Cs4CuSb2Cl12. *Physical Review B*, **2020**, 101,	3.3	9
22	Performance of SCAN density functional for a set of ionic liquid ion pairs. *International Journal of Quantum Chemistry*, **2018**, 118, e25582	2.1	9
21	Extension to Negative Values of the Coupling Constant of Adiabatic Connection for Interaction-Strength Interpolation. *Journal of Chemical Theory and Computation*, **2009**, 5, 708-11	6.4	9
20	Tunable catalytic activity of cobalt-intercalated layered MnO2 for water oxidation through confinement and local ordering. *Journal of Catalysis*, **2019**, 374, 143-149	7.3	8
19	High yield production of ultrathin fibroid semiconducting nanowire of Ta2Pd3Se8. *Nano Research*, **2020**, 13, 1627-1635	10	8
18	Exceptionally large anomalous Hall effect due to anticrossing of spin-split bands in the antiferromagnetic half-Heusler compound TbPtBi. *Physical Review B*, **2020**, 101,	3.3	8
17	Density functional theory **2019**, 119-159		7
16	Structural and Electronic Transport Properties of Fluorographene Directly Grown on Silicates for Possible Biosensor Applications. *ACS Applied Nano Materials*, **2020**, 3, 5399-5409	5.6	6
15	The two pillars: density and spin-density functional theories. *Molecular Physics*, **2016**, 114, 928-931	1.7	6
14	Composition-induced type I and direct bandgap transition metal dichalcogenides alloy vertical heterojunctions. *Nanoscale*, **2020**, 12, 201-209	7.7	6
13	Bonding in the metallic molecular solid Gallium. *Molecular Physics*, **2018**, 116, 3372-3379	1.7	6
12	Understanding the Boron-Nitrogen Interaction and Its Possible Implications in Drug Design. *Journal of Physical Chemistry B*, **2015**, 119, 14393-401	3.4	5
11	Examining the order-of-limits problem and lattice constant performance of the Tao-Mo functional. *Journal of Chemical Physics*, **2020**, 152, 244112	3.9	5
10	Construction of meta-GGA functionals through restoration of exact constraint adherence to regularized SCAN functionals.. *Journal of Chemical Physics*, **2022**, 156, 034109	3.9	5
9	Subtle metastability of the layered magnetic topological insulator MnBi2Te4 from weak interactions. *Npj Computational Materials*, **2020**, 6,	10.9	5
8	Spin-valley locking and bulk quantum Hall effect in a noncentrosymmetric Dirac semimetal BaMnSb. *Nature Communications*, **2021**, 12, 4062	17.4	4
7	Ab initio description of the Bi2Sr2CaCu2O8+ electronic structure. *Physical Review B*, **2020**, 101,	3.3	3

6	Magnetic oxygen in transition metal oxides: A case study of Ba2CoO4. *Journal of Physics and Chemistry of Solids*, **2021**, 150, 109803	3.9	1
5	Egyptian blue: from pigment to battery electrodes.. *RSC Advances*, **2021**, 11, 19885-19889	3.7	1
4	Reliable Lattice Dynamics from an Efficient Density Functional Approximation. *Chemistry of Materials*, **2022**, 34, 2562-2568	9.6	1
3	Transition Metal Carbo-Chalcogenide "TMCC" a New Family of Two-dimensional Materials.. *Advanced Materials*, **2022**, e2200574	24	1
2	Comparative first-principles study of elastic constants of covalent and ionic materials with LDA, GGA, and meta-GGA functionals and the prediction of mechanical hardness. *Science China Technological Sciences*,1	3.5	0
1	Decoding defect ordering from ADF-STEM images of van der Waals CrGa2Te7 ferromagnetic crystals using the unsupervised machine learning algorithm. *Microscopy and Microanalysis*, **2021**, 27, 710-711	0.5	