Jianwei Sun

List of Publications by Year in descending order

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83	9,335	76196 40	58464 82
papers	citations	h-index	g-index

89	89	89	8219
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Strongly Constrained and Appropriately Normed Semilocal Density Functional. Physical Review Letters, 2015, 115, 036402.	2.9	2,273
2	Density functional theory is straying from the path toward the exact functional. Science, 2017, 355, 49-52.	6.0	711
3	Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. Nature Chemistry, 2016, 8, 831-836.	6.6	698
4	Workhorse Semilocal Density Functional for Condensed Matter Physics and Quantum Chemistry. Physical Review Letters, 2009, 103, 026403.	2.9	507
5	Understanding band gaps of solids in generalized Kohnâ€“Sham theory. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2801-2806.	3.3	423
6	Accurate and Numerically Efficient r²SCAN Meta-Generalized Gradient Approximation. Journal of Physical Chemistry Letters, 2020, 11, 8208-8215.	2.1	335
7	Versatile van der Waals Density Functional Based on a Meta-Generalized Gradient Approximation. Physical Review X, 2016, 6, .	2.8	321
8	Some Fundamental Issues in Ground-State Density Functional Theory: A Guide for the Perplexed. Journal of Chemical Theory and Computation, 2009, 5, 902-908.	2.3	306
9	Energetics of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MnO</mml:mi><mml:mn>2</mml:mn></mml:msub></mm in density functional theory. Physical Review B, 2016, 93, .	1.1	204
10	More realistic band gaps from meta-generalized gradient approximations: Only in a generalized Kohn-Sham scheme. Physical Review B, 2016, 93, .	1.1	182
11	Self-consistent meta-generalized gradient approximation within the projector-augmented-wave method. Physical Review B, 2011, 84, .	1.1	180
12	Density Functionals that Recognize Covalent, Metallic, and Weak Bonds. Physical Review Letters, 2013, 111, 106401.	2.9	168
13	Semilocal and hybrid meta-generalized gradient approximations based on the understanding of the kinetic-energy-density dependence. Journal of Chemical Physics, 2013, 138, 044113.	1.2	164
14	Efficient first-principles prediction of solid stability: Towards chemical accuracy. Npj Computational Materials, 2018, 4, .	3.5	157
15	Comparative first-principles studies of prototypical ferroelectric materials by LDA, GGA, and SCAN meta-GGA. Physical Review B, 2017, 96, .	1.1	156
16	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.	3.3	152
17	Communication: Effect of the orbital-overlap dependence in the meta generalized gradient approximation. Journal of Chemical Physics, 2012, 137, 051101.	1.2	122
18	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, 685-689.	3.3	119

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19	van der Waals bilayer energetics: Generalized stacking-fault energy of graphene, boron nitride, and graphene/boron nitride bilayers. Physical Review B, 2015, 92, .	1.1	105
20	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, .	1.1	100
21	An accurate first-principles treatment of doping-dependent electronic structure of high-temperature cuprate superconductors. Communications Physics, 2018, 1, .	2.0	94
22	Testing density functionals for structural phase transitions of solids under pressure: Si, SiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>, and Zr. Physical Review B, 2013, 88, .	1.1	87
23	Gedanken densities and exact constraints in density functional theory. Journal of Chemical Physics, 2014, 140, 18A533.	1.2	82
24	Antiferromagnetic ground state of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>La</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>: A parameter-free ab initio description. Physical Review B, 2018, 98, .	1.1	80
25	r2SCAN-D4: Dispersion corrected meta-generalized gradient approximation for general chemical applications. Journal of Chemical Physics, 2021, 154, 061101.	1.2	70
26	Copper-Intercalated Birnessite as a Water Oxidation Catalyst. Langmuir, 2015, 31, 12807-12813.	1.6	69
27	Performance of meta-GGA Functionals on General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2013, 9, 355-363.	2.3	68
28	Improved lattice constants, surface energies, and CO desorption energies from a semilocal density functional. Physical Review B, 2011, 83, .	1.1	67
29	Semilocal density functionals and constraint satisfaction. International Journal of Quantum Chemistry, 2016, 116, 847-851.	1.0	65
30	Lattice constants from semilocal density functionals with zero-point phonon correction. Physical Review B, 2012, 85, .	1.1	63
31	First-Principles Prediction of a Stable Hexagonal Phase of CH₃NH₃PbI₃. Chemistry of Materials, 2017, 29, 6003-6011.	3.2	62
32	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.	3.3	61
33	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, .	3.3	53
34	Correlation energy of the uniform electron gas from an interpolation between high- and low-density limits. Physical Review B, 2010, 81, .	1.1	51
35	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, .	1.1	51
36	Response to Comment on â€œDensity functional theory is straying from the path toward the exact functionalâ€• Science, 2017, 356, 496-496.	6.0	51

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37	A meta-GGA Made Free of the Order of Limits Anomaly. Journal of Chemical Theory and Computation, 2012, 8, 2078-2087.	2.3	49
38	Symmetry-breaking polymorphous descriptions for correlated materials without interelectronic U. Physical Review B, 2020, 102, .	1.1	48
39	Rethinking CO adsorption on transition-metal surfaces: Effect of density-driven self-interaction errors. Physical Review B, 2019, 100, .	1.1	44
40	Water Oxidation Catalyzed by Cobalt Oxide Supported on the Mattagamite Phase of CoTe₂. ACS Catalysis, 2016, 6, 7393-7397.	5.5	39
41	Magnetic and f-electron effects in LaNiO2 and NdNiO2 nickelates with cuprate-like $$3{d}_{{x}^{2}-{y}^{2}}$$ band. Communications Physics, 2021, 4, .	2.0	38
42	Enhancing the efficiency of density functionals with an improved iso-orbital indicator. Physical Review B, 2019, 99, .	1.1	37
43	Subtlety of TiO2 phase stability: Reliability of the density functional theory predictions and persistence of the self-interaction error. Journal of Chemical Physics, 2019, 150, 014105.	1.2	32
44	Spin-valley locking and bulk quantum Hall effect in a noncentrosymmetric Dirac semimetal BaMnSb2. Nature Communications, 2021, 12, 4062.	5.8	32
45	Adsorption and Deposition of Li₂O₂ on TiC{111} Surface. Journal of Physical Chemistry Letters, 2014, 5, 3919-3923.	2.1	30
46	Coulomb correlation in noncollinear antiferromagnetic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi></mml:math> -Mn. Physical Review B, 2020, 101, .	1.1	27
47	Accurate, Precise, and Efficient Theoretical Methods To Calculate Anionâ^'Ï€ Interaction Energies in Model Structures. Journal of Chemical Theory and Computation, 2015, 11, 360-371.	2.3	26
48	Dependence of the structure and dynamics of liquid silicon on the choice of density functional approximation. Physical Review B, 2017, 96, .	1.1	26
49	Structural phase transitions in Si and SiO2crystals via the random phase approximation. Physical Review B, 2012, 86, .	1.1	25
50	Construction of meta-GGA functionals through restoration of exact constraint adherence to regularized SCAN functionals. Journal of Chemical Physics, 2022, 156, 034109.	1.2	25
51	Exceptionally large anomalous Hall effect due to anticrossing of spin-split bands in the antiferromagnetic half-Heusler compound TbPtBi. Physical Review B, 2020, 101, .	1.1	24
52	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.	0.8	23
53	First-principles calculation of spin and orbital contributions to magnetically ordered moments in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sr</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mr Physical Review B, 2020, 101, .	1.1	23
54	Communication: Near-locality of exchange and correlation density functionals for 1- and 2-electron systems. Journal of Chemical Physics, 2016, 144, 191101.	1.2	20

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55	Why Density Functionals Should Not Be Judged Primarily by Atomization Energies. Periodica Polytechnica: Chemical Engineering, 2016, 60, 2-7.	0.5	18
56	Transition Metal Carboâ€Chalcogenide â€œTMCC:â€•A New Family of 2D Materials. Advanced Materials, 2022, 34, e2200574.	11.1	18
57	High yield production of ultrathin fibroid semiconducting nanowire of Ta2Pd3Se8. Nano Research, 2020, 13, 1627-1635.	5.8	16
58	van der Waals interaction as a summable asymptotic series. Physical Review A, 2012, 86, .	1.0	15
59	Composition-induced type I and direct bandgap transition metal dichalcogenides alloy vertical heterojunctions. Nanoscale, 2020, 12, 201-209.	2.8	15
60	Intensive Atomization Energy: Re-Thinking a Metric for Electronic Structure Theory Methods. Zeitschrift Fur Physikalische Chemie, 2016, 230, 737-742.	1.4	14
61	Spinon excitations in the quasi-one-dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>S</mml:mi><mml:mo>=</mml:mo><mml:mfrac><mml:m chain compound <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">s</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:mi>CuS</mml:mi><mml:msub><mml:mi mathvariant="normal">b</mml:mi><mml:mn>. Physical Review B, 2020, 101, .	1.1	14
62	Extension to Negative Values of the Coupling Constant of Adiabatic Connection for Interaction-Strength Interpolation. Journal of Chemical Theory and Computation, 2009, 5, 708-711.	2.3	13
63	Tunable catalytic activity of cobalt-intercalated layered MnO2 for water oxidation through confinement and local ordering. Journal of Catalysis, 2019, 374, 143-149.	3.1	13
64	Sensitivity of the electronic and magnetic structures of cuprate superconductors to density functional approximations. Npj Computational Materials, 2022, 8, .	3.5	12
65	Reliable Lattice Dynamics from an Efficient Density Functional Approximation. Chemistry of Materials, 2022, 34, 2562-2568.	3.2	12
66	Examining the order-of-limits problem and lattice constant performance of the Taoâ€“Mo functional. Journal of Chemical Physics, 2020, 152, 244112.	1.2	11
67	Ab initio description of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Bi</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:m mathvariant="normal">O</mml:mi><mml:mrow><mml:mn>8</mml:mn><mml:mo>+</mml:mo><mml:mi>Î´</mml:mi></mml:mrow></m electronic structure. Physical Review B, 2020, 101, .	1.1	11
68	Ferromagnetic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>MnBi</mml:mi><mml:mn>4</mml:mn></mml:m obtained with low-concentration Sb doping: A promising platform for exploring topological quantum states. Physical Review Materials, 2022, 6, .	0.9	11
69	Performance of SCAN density functional for a set of ionic liquid ion pairs. International Journal of Quantum Chemistry, 2018, 118, e25582.	1.0	10
70	Subtle metastability of the layered magnetic topological insulator MnBi2Te4 from weak interactions. Npj Computational Materials, 2020, 6, .	3.5	8
71	Structural and Electronic Transport Properties of Fluorographene Directly Grown on Silicates for Possible Biosensor Applications. ACS Applied Nano Materials, 2020, 3, 5399-5409.	2.4	8
72	Bonding in the metallic molecular solid Î±-Gallium. Molecular Physics, 2018, 116, 3372-3379.	0.8	7

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73	Density functional theory. , 2019, , 119-159.		7
74	The two pillars: density and spin-density functional theories. Molecular Physics, 2016, 114, 928-931.	0.8	6
75	Critical role of magnetic moments in heavy-fermion materials: Revisiting <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>SmB</mml:mi></mml:mrow><mml:mn>6</mml:mn> Physical Review B, 2022, 105, .	1.1	6
76	Understanding the Boronâ€“Nitrogen Interaction and Its Possible Implications in Drug Design. Journal of Physical Chemistry B, 2015, 119, 14393-14401.	1.2	5
77	Weyl semimetal in the rare-earth hexaboride family supporting a pseudonodal surface and a giant anomalous Hall effect. Physical Review B, 2022, 105, .	1.1	4
78	Egyptian blue: from pigment to battery electrodes. RSC Advances, 2021, 11, 19885-19889.	1.7	3
79	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, 2021, 64, 2755-2761.	2.0	3
80	Magnetic oxygen in transition metal oxides: A case study of Ba2CoO4. Journal of Physics and Chemistry of Solids, 2021, 150, 109803.	1.9	2
81	(Invited) SCAN Meta-GGA: An Accurate, Efficient, and Physically Sound Density Functional for Materials Discovery and Design. ECS Meeting Abstracts, 2019, , .	0.0	1
82	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.	0.2	0
83	Application of wavefunction methods to metals. Nature Computational Science, 2021, 1, 780-781.	3.8	0