

Jianmin Tao

List of Publications by Year in descending order

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papers

11,385
citations

218381

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58
times ranked

8861
citing authors

#	ARTICLE	IF	CITATIONS
1	Climbing the Density Functional Ladder: Nonempirical Meta-“Generalized Gradient Approximation Designed for Molecules and Solids. <i>Physical Review Letters</i> , 2003, 91, 146401.	2.9	5,673
2	Comparative assessment of a new nonempirical density functional: Molecules and hydrogen-bonded complexes. <i>Journal of Chemical Physics</i> , 2003, 119, 12129-12137.	1.2	2,157
3	Prescription for the design and selection of density functional approximations: More constraint satisfaction with fewer fits. <i>Journal of Chemical Physics</i> , 2005, 123, 062201.	1.2	769
4	Meta-generalized gradient approximation: Explanation of a realistic nonempirical density functional. <i>Journal of Chemical Physics</i> , 2004, 120, 6898-6911.	1.2	431
5	Tests of a ladder of density functionals for bulk solids and surfaces. <i>Physical Review B</i> , 2004, 69, .	1.1	349
6	Density functional with full exact exchange, balanced nonlocality of correlation, and constraint satisfaction. <i>Physical Review A</i> , 2008, 78, .	1.0	221
7	Accurate Semilocal Density Functional for Condensed-Matter Physics and Quantum Chemistry. <i>Physical Review Letters</i> , 2016, 117, 073001.	2.9	124
8	Exact-exchange energy density in the gauge of a semilocal density-functional approximation. <i>Physical Review A</i> , 2008, 77, .	1.0	104
9	Test of a nonempirical density functional: Short-range part of the van der Waals interaction in rare-gas dimers. <i>Journal of Chemical Physics</i> , 2005, 122, 114102.	1.2	103
10	Accurate van der Waals coefficients from density functional theory. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 18-21.	3.3	77
11	Meta-generalized gradient approximation for the exchange-correlation hole with an application to the jellium surface energy. <i>Physical Review B</i> , 2006, 73, .	1.1	71
12	Performance of meta-GGA Functionals on General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 355-363.	2.3	68
13	Van der Waals Coefficients for Nanostructures: Fullerenes Defy Conventional Wisdom. <i>Physical Review Letters</i> , 2012, 109, 233203.	2.9	66
14	Long-range van der Waals attraction and alkali-metal lattice constants. <i>Physical Review B</i> , 2010, 81, .	1.1	65
15	Energies of organic molecules and atoms in density functional theory. <i>International Journal of Quantum Chemistry</i> , 2005, 101, 506-511.	1.0	64
16	Nonempirical Construction of Current-Density Functionals from Conventional Density-Functional Approximations. <i>Physical Review Letters</i> , 2005, 95, 196403.	2.9	61
17	Physical Adsorption: Theory of van der Waals Interactions between Particles and Clean Surfaces. <i>Physical Review Letters</i> , 2014, 112, 106101.	2.9	54
18	How correlation suppresses density fluctuations in the uniform electron gas of one, two, or three dimensions. <i>International Journal of Quantum Chemistry</i> , 2000, 77, 819-830.	1.0	40

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19	Origin of the size-dependence of the equilibrium van der Waals binding between nanostructures. <i>Journal of Chemical Physics</i> , 2018, 148, 074110.	1.2	39
20	One-parameter optimization of a nonempirical meta-generalized-gradient-approximation for the exchange-correlation energy. <i>Physical Review A</i> , 2007, 76, .	1.0	37
21	Assessment of the Tao-Mo nonempirical semilocal density functional in applications to solids and surfaces. <i>Physical Review B</i> , 2017, 95, .	1.1	37
22	Performance of a nonempirical meta-generalized gradient approximation density functional for excitation energies. <i>Journal of Chemical Physics</i> , 2008, 128, 084110.	1.2	32
23	Uniform electron gas from the Colle-Salvetti functional: Missing long-range correlations. <i>Physical Review A</i> , 2001, 63, .	1.0	31
24	Exchange energy density of an atom as a functional of the electron density. <i>Journal of Chemical Physics</i> , 2001, 115, 3519-3530.	1.2	28
25	Ice phases under ambient and high pressure: Insights from density functional theory. <i>Physical Review B</i> , 2013, 87, .	1.1	28
26	Visualizing atomic sizes and molecular shapes with the classical turning surface of the Kohn-Sham potential. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E11578-E11585.	3.3	27
27	Properties of the exchange hole under an appropriate coordinate transformation. <i>Journal of Chemical Physics</i> , 2003, 119, 6457-6464.	1.2	26
28	Performance of a nonempirical density functional on molecules and hydrogen-bonded complexes. <i>Journal of Chemical Physics</i> , 2016, 145, 234306.	1.2	25
29	Frequency-dependent dielectric function of semiconductors with application to physisorption. <i>Physical Review B</i> , 2017, 95, .	1.1	25
30	Communication: Non-additivity of van der Waals interactions between nanostructures. <i>Journal of Chemical Physics</i> , 2014, 141, 141101.	1.2	24
31	Communication: Accurate higher-order van der Waals coefficients between molecules from a model dynamic multipole polarizability. <i>Journal of Chemical Physics</i> , 2016, 144, 031102.	1.2	22
32	An accurate MGGA-based hybrid exchange-correlation functional. <i>Journal of Chemical Physics</i> , 2002, 116, 2335-2337.	1.2	20
33	Performance of a nonempirical exchange functional from density matrix expansion: comparative study with different correlations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21707-21713.	1.3	20
34	Semilocal exchange hole with an application to range-separated density functionals. <i>Physical Review B</i> , 2017, 95, .	1.1	19
35	Screened van der Waals correction to density functional theory for solids. <i>Physical Review Materials</i> , 2017, 1, .	0.9	19
36	van der Waals Correction to the Physisorption of Graphene on Metal Surfaces. <i>Journal of Physical Chemistry C</i> , 2019, 123, 13748-13757.	1.5	18

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37	Dynamical screening of van der Waals interactions in nanostructured solids: Sublimation of fullerenes. <i>Journal of Chemical Physics</i> , 2015, 142, 164302.	1.2	15
38	Modeling the physisorption of graphene on metals. <i>Physical Review B</i> , 2018, 97, .	1.1	15
39	Accurate lattice geometrical parameters and bulk moduli from a semilocal density functional. <i>AIP Advances</i> , 2018, 8, .	0.6	15
40	LONG-RANGE VAN DER WAALS INTERACTION. <i>International Journal of Modern Physics B</i> , 2013, 27, 1330011.	1.0	14
41	First-principles study of the binding energy between nanostructures and its scaling with system size. <i>Physical Review B</i> , 2018, 97, .	1.1	13
42	Spherical-shell model for the van der Waals coefficients between fullerenes and/or nearly spherical nanoclusters. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 424207.	0.7	12
43	Accurate van der Waals coefficients between fullerenes and fullerene-alkali atoms and clusters: Modified single-frequency approximation. <i>Physical Review B</i> , 2016, 94, .	1.1	12
44	Comparative study of semilocal density functionals on solids and surfaces. <i>Chemical Physics Letters</i> , 2017, 682, 38-42.	1.2	12
45	Accurate excitation energies of molecules and oligomers from a semilocal density functional. <i>Journal of Chemical Physics</i> , 2017, 146, 234102.	1.2	11
46	Van der Waals coefficients beyond the classical shell model. <i>Journal of Chemical Physics</i> , 2015, 142, 024312.	1.2	8
47	Quantum pressure and chemical bonding: Influence of magnetic fields on electron localization. <i>Physical Review B</i> , 2015, 92, .	1.1	8
48	Comparative study of the properties of ionic solids from density functionals. <i>Materials Research Express</i> , 2018, 5, 076302.	0.8	8
49	Density functionals combined with van der Waals corrections for graphene adsorbed on layered materials. <i>Physical Review B</i> , 2020, 101, .	1.1	8
50	Energetic Study of Clusters and Reaction Barrier Heights from Efficient Semilocal Density Functionals. <i>Computation</i> , 2017, 5, 27.	1.0	7
51	Uniform Density Limit of Exchange-Correlation Energy Functionals. <i>ACS Symposium Series</i> , 2007, , 13-25.	0.5	5
52	Long-range dispersion-corrected density functional for noncovalent interactions. <i>International Journal of Modern Physics B</i> , 2019, 33, 1950300.	1.0	5
53	CORRELATION ENERGY DENSITIES: E PLURIBUS UNUM. , 2002, , 719-730.		1
54	Geometric Derivation of the Stress Tensor of the Homogeneous Electron Gas. <i>Computation</i> , 2017, 5, 28.	1.0	1

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55	Exchange-correlation energies of atoms from efficient density functionals: influence of the electron density. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2017, 50, 245004.	0.6	0