Jianmin Tao

List of Publications by Year
in descending order

55 papers	11,385 citations	218677 26 h-index	149698 56 g-index
58 all docs	58 docs citations	58 times ranked	8861 citing authors

#	Article	IF	Citations
1	Climbing the Density Functional Ladder: Nonempirical Metaâ€“Generalized Gradient Approximation Designed for Molecules and Solids. Physical Review Letters, 2003, 91, 146401.	7.8	5,673
2	Comparative assessment of a new nonempirical density functional: Molecules and hydrogen-bonded complexes. Journal of Chemical Physics, 2003, 119, 12129-12137.	3.0	2,157
3	Prescription for the design and selection of density functional approximations: More constraint satisfaction with fewer fits. Journal of Chemical Physics, 2005, 123, 062201.	3.0	769
4	Meta-generalized gradient approximation: Explanation of a realistic nonempirical density functional. Journal of Chemical Physics, 2004, 120, 6898-6911.	3.0	431
5	Tests of a ladder of density functionals for bulk solids and surfaces. Physical Review B, 2004, 69, .	3.2	349
6	Density functional with full exact exchange, balanced nonlocality of correlation, and constraint satisfaction. Physical Review A, 2008, 78, .	2.5	221
7	Accurate Semilocal Density Functional for Condensed-Matter Physics and Quantum Chemistry. Physical Review Letters, 2016, 117, 073001.	7.8	124
8	Exact-exchange energy density in the gauge of a semilocal density-functional approximation. Physical Review A, 2008, 77, .	2.5	104
9	Test of a nonempirical density functional: Short-range part of the van der Waals interaction in rare-gas dimers. Journal of Chemical Physics, 2005, 122, 114102.	3.0	103
10	Accurate van der Waals coefficients from density functional theory. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 18-21.	7.1	77
11	Meta-generalized gradient approximation for the exchange-correlation hole with an application to the jellium surface energy. Physical Review B, 2006, 73, .	3.2	71
12	Performance of meta-GGA Functionals on General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2013, 9, 355-363.	5.3	68
13	Van der Waals Coefficients for Nanostructures: Fullerenes Defy Conventional Wisdom. Physical Review Letters, 2012, 109, 233203.	7.8	66
14	Long-range van der Waals attraction and alkali-metal lattice constants. Physical Review B, 2010, 81, .	3.2	65
15	Energies of organic molecules and atoms in density functional theory. International Journal of Quantum Chemistry, 2005, 101, 506-511.	2.0	64
16	Nonempirical Construction of Current-Density Functionals from Conventional Density-Functional Approximations. Physical Review Letters, 2005, 95, 196403.	7.8	61
17	Physical Adsorption: Theory of van der Waals Interactions between Particles and Clean Surfaces. Physical Review Letters, 2014, 112, 106101.	7.8	54
18	How correlation suppresses density fluctuations in the uniform electron gas of one, two, or three dimensions. International Journal of Quantum Chemistry, 2000, 77, 819-830.	2.0	40

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19	Origin of the size-dependence of the equilibrium van der Waals binding between nanostructures. Journal of Chemical Physics, 2018, 148, 074110.	3.0	39
20	One-parameter optimization of a nonempirical meta-generalized-gradient-approximation for the exchange-correlation energy. Physical Review A, 2007, 76, .	2.5	37
21	Assessment of the Tao-Mo nonempirical semilocal density functional in applications to solids and surfaces. Physical Review B, 2017, 95, .	3.2	37
22	Performance of a nonempirical metaâ€“generalized gradient approximation density functional for excitation energies. Journal of Chemical Physics, 2008, 128, 084110.	3.0	32
23	Uniform electron gas from the Colle-Salvetti functional: Missing long-range correlations. Physical Review A, 2001, 63, .	2.5	31
24	Exchange energy density of an atom as a functional of the electron density. Journal of Chemical Physics, 2001, 115, 3519-3530.	3.0	28
25	Ice phases under ambient and high pressure: Insights from density functional theory. Physical Review B, 2013, 87, .	3.2	28
26	Visualizing atomic sizes and molecular shapes with the classical turning surface of the Kohnâ€“Sham potential. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E11578-E11585.	7.1	27
27	Properties of the exchange hole under an appropriate coordinate transformation. Journal of Chemical Physics, 2003, 119, 6457-6464.	3.0	26
28	Performance of a nonempirical density functional on molecules and hydrogen-bonded complexes. Journal of Chemical Physics, 2016, 145, 234306.	3.0	25
29	Frequency-dependent dielectric function of semiconductors with application to physisorption. Physical Review B, 2017, 95, .	3.2	25
30	Communication: Non-additivity of van der Waals interactions between nanostructures. Journal of Chemical Physics, 2014, 141, 141101.	3.0	24
31	Communication: Accurate higher-order van der Waals coefficients between molecules from a model dynamic multipole polarizability. Journal of Chemical Physics, 2016, 144, 031102.	3.0	22
32	An accurate MGGA-based hybrid exchange-correlation functional. Journal of Chemical Physics, 2002, 116, 2335-2337.	3.0	20
33	Performance of a nonempirical exchange functional from density matrix expansion: comparative study with different correlations. Physical Chemistry Chemical Physics, 2017, 19, 21707-21713.	2.8	20
34	Semilocal exchange hole with an application to range-separated density functionals. Physical Review B, 2017, 95, .	3.2	19
35	Screened van der Waals correction to density functional theory for solids. Physical Review Materials, 2017, 1, .	2.4	19
36	van der Waals Correction to the Physisorption of Graphene on Metal Surfaces. Journal of Physical Chemistry C, 2019, 123, 13748-13757.	3.1	18

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37	Dynamical screening of van der Waals interactions in nanostructured solids: Sublimation of fullerenes. Journal of Chemical Physics, 2015, 142, 164302.	3.0	15
38	Modeling the physisorption of graphene on metals. Physical Review B, 2018, 97, .	3.2	15
39	Accurate lattice geometrical parameters and bulk moduli from a semilocal density functional. AIP Advances, 2018, 8, .	1.3	15
40	LONG-RANGE VAN DER WAALS INTERACTION. International Journal of Modern Physics B, 2013, 27, 1330011.	2.0	14
41	First-principles study of the binding energy between nanostructures and its scaling with system size. Physical Review B, 2018, 97, .	3.2	13
42	Spherical-shell model for the van der Waals coefficients between fullerenes and/or nearly spherical nanoclusters. Journal of Physics Condensed Matter, 2012, 24, 424207.	1.8	12
43	Accurate van der Waals coefficients between fullerenes and fullerene-alkali atoms and clusters: Modified single-frequency approximation. Physical Review B, 2016, 94, .	3.2	12
44	Comparative study of semilocal density functionals on solids and surfaces. Chemical Physics Letters, 2017, 682, 38-42.	2.6	12
45	Accurate excitation energies of molecules and oligomers from a semilocal density functional. Journal of Chemical Physics, 2017, 146, 234102.	3.0	11
46	Van der Waals coefficients beyond the classical shell model. Journal of Chemical Physics, 2015, 142, 024312.	3.0	8
47	Quantum pressure and chemical bonding: Influence of magnetic fields on electron localization. Physical Review B, 2015, 92, .	3.2	8
48	Comparative study of the properties of ionic solids from density functionals. Materials Research Express, 2018, 5, 076302.	1.6	8
49	Density functionals combined with van der Waals corrections for graphene adsorbed on layered materials. Physical Review B, 2020, 101, .	3.2	8
50	Energetic Study of Clusters and Reaction Barrier Heights from Efficient Semilocal Density Functionals. Computation, 2017, 5, 27.	2.0	7
51	Uniform Density Limit of Exchange-Correlation Energy Functionals. ACS Symposium Series, 2007, , 13-25.	0.5	5
52	Long-range dispersion-corrected density functional for noncovalent interactions. International Journal of Modern Physics B, 2019, 33, 1950300.	2.0	5
53	CORRELATION ENERGY DENSITIES: E PLURIBUS UNUM. , 2002, , 719-730.		1
54	Geometric Derivation of the Stress Tensor of the Homogeneous Electron Gas. Computation, 2017, 5, 28.	2.0	1

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55	Exchange-correlation energies of atoms from efficient density functionals: influence of the electron density. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 245004.	1.5	0