Jeng-Da Chai

List of Publications by Year
in descending order

63 papers	19,415 citations	147726 31 h-index	114418 63 g-index
63 all docs	63 docs citations	63 times ranked	17789 citing authors

#	Article	IF	Citations
1	Long-range corrected hybrid density functionals with damped atomâ€“atom dispersion corrections. Physical Chemistry Chemical Physics, 2008, 10, 6615.	1.3	10,464
2	Systematic optimization of long-range corrected hybrid density functionals. Journal of Chemical Physics, 2008, 128, 084106.	1.2	2,890
3	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
4	Long-Range Corrected Hybrid Density Functionals with Improved Dispersion Corrections. Journal of Chemical Theory and Computation, 2013, 9, 263-272.	2.3	535
5	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
6	Long-range corrected double-hybrid density functionals. Journal of Chemical Physics, 2009, 131, 174105.	1.2	327
7	Impact of Metal and Anion Substitutions on the Hydrogen Storage Properties of M-BTT Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2013, 135, 1083-1091.	6.6	139
8	Density functional theory with fractional orbital occupations. Journal of Chemical Physics, 2012, 136, 154104.	1.2	127
9	SCAN-based hybrid and double-hybrid density functionals from models without fitted parameters. Journal of Chemical Physics, 2016, 144, 044114.	1.2	126
10	Semiempirical Double-Hybrid Density Functional with Improved Description of Long-Range Correlation. Journal of Physical Chemistry A, 2008, 112, 2702-2712.	1.1	123
11	Seeking for reliable double-hybrid density functionals without fitting parameters: The PBE0-2 functional. Chemical Physics Letters, 2012, 538, 121-125.	1.2	118
12	Long-range corrected hybrid meta-generalized-gradient approximations with dispersion corrections. Journal of Chemical Physics, 2012, 136, 154109.	1.2	101
13	Thermoelectric properties, phonon, and mechanical stability of new half-metallic quaternary Heusler alloys: FeRhCrZ (Zâ€‰=â€‰Si and Ge). Journal of Applied Physics, 2020, 127, .	1.1	90
14	Electronic Properties of Zigzag Graphene Nanoribbons Studied by TAO-DFT. Journal of Chemical Theory and Computation, 2015, 11, 2003-2011.	2.3	69
15	Optimal operators for Hartreeâ€“Fock exchange from long-range corrected hybrid density functionals. Chemical Physics Letters, 2008, 467, 176-178.	1.2	68
16	Thermally-assisted-occupation density functional theory with generalized-gradient approximations. Journal of Chemical Physics, 2014, 140, 18A521.	1.2	64
17	Role of KekulÃ© and Non-KekulÃ© Structures in the Radical Character of Alternant Polycyclic Aromatic Hydrocarbons: A TAO-DFT Study. Scientific Reports, 2016, 6, 30562.	1.6	63
18	Strain engineering of electronic structure, phonon, and thermoelectric properties of p-type half-Heusler semiconductor. Journal of Alloys and Compounds, 2021, 850, 156615.	2.8	51

#	Article	IF	Citations
19	Electronic Properties of Cyclacenes from TAO-DFT. Scientific Reports, 2016, 6, 37249.	1.6	50
20	Assessment of density functional methods with correct asymptotic behavior. Physical Chemistry Chemical Physics, 2013, 15, 8352.	1.3	49
21	Assessment of density functional methods for exciton binding energies and related optoelectronic properties. RSC Advances, 2015, 5, 101370-101376.	1.7	47
22	Restoration of the Derivative Discontinuity in Kohn-Sham Density Functional Theory: An Efficient Scheme for Energy Gap Correction. Physical Review Letters, 2013, 110, 033002.	2.9	46
23	Effect of Li Adsorption on the Electronic and Hydrogen Storage Properties of Acenes: A Dispersion-Corrected TAO-DFT Study. Scientific Reports, 2016, 6, 33081.	1.6	46
24	Novel half-metallic L21 structured full-Heusler compound for promising spintronic applications: A DFT-based computer simulation. Journal of Magnetism and Magnetic Materials, 2019, 487, 165289.	1.0	43
25	Assessment of density functional approximations for the hemibonded structure of the water dimer radical cation. Physical Chemistry Chemical Physics, 2012, 14, 10705.	1.3	41
26	Orbital-free density functional theory: Kinetic potentials andab initiolocal pseudopotentials. Physical Review B, 2007, 75, .	1.1	38
27	Role of exact exchange in thermally-assisted-occupation density functional theory: A proposal of new hybrid schemes. Journal of Chemical Physics, 2017, 146, 044102.	1.2	38
28	Dynamic structure factor of liquid and amorphous Ge fromab initiosimulations. Physical Review B, 2003, 67, .	1.1	37
29	Robust stability, half-metallic ferrimagnetism and thermoelectric properties of new quaternary Heusler material: A first principles approach. Journal of Magnetism and Magnetic Materials, 2020, 502, 166562.	1.0	36
30	Self-consistent determination of the fictitious temperature in thermally-assisted-occupation density functional theory. RSC Advances, 2017, 7, 50496-50507.	1.7	33
31	Electronic and Hydrogen Storage Properties of Li-Terminated Linear Boron Chains Studied by TAO-DFT. Scientific Reports, 2018, 8, 13538.	1.6	32
32	Origin of pseudo gap and thermoelectric signatures of semimetallic Ru2TaGa: Structural stability from phonon dynamics, mechanical, and thermodynamic predictions. Journal of Physics and Chemistry of Solids, 2021, 154, 110098.	1.9	28
33	Effect of Li Termination on the Electronic and Hydrogen Storage Properties of Linear Carbon Chains: A TAO-DFT Study. Scientific Reports, 2017, 7, 4966.	1.6	27
34	Short- and long-range corrected hybrid density functionals with the D3 dispersion corrections. Journal of Chemical Physics, 2016, 145, 204101.	1.2	26
35	TAO-DFT investigation of electronic properties of linear and cyclic carbon chains. Scientific Reports, 2020, 10, 13133.	1.6	26
36	Modified Statistical Treatment of Kinetic Energy in the Thomasâ˜'Fermi Model. Journal of Physical Chemistry B, 2004, 108, 6870-6876.	1.2	24

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37	Electronic Properties of MÃ¶bius Cyclacenes Studied by Thermally-Assisted-Occupation Density Functional Theory. Scientific Reports, 2019, 9, 2907.	1.6	23
38	Synthesis, characterization, antimicrobial, BSA binding, DFT calculation, molecular docking and cytotoxicity of Ni(II) complexes with Schiff base ligands. Journal of Molecular Liquids, 2021, 328, 115457.	2.3	22
39	Electronic properties of the coronene series from thermally-assisted-occupation density functional theory. RSC Advances, 2018, 8, 34350-34358.	1.7	21
40	Electronic Properties of Triangle-Shaped Graphene Nanoflakes from TAO-DFT. ACS Omega, 2019, 4, 14202-14210.	1.6	18
41	Orbital-free density functional theory: Linear scaling methods for kinetic potentials, and applications to solid Al and Si. Chemical Physics Letters, 2009, 473, 263-267.	1.2	17
42	Growth and characterization of crystalline BaSnO3 perovskite nanostructures and the influence of heavy Mn doping on its properties. Journal of Alloys and Compounds, 2021, 867, 158900.	2.8	17
43	Local Density Approximation for the Short-Range Exchange Free Energy Functional. ACS Omega, 2019, 4, 7675-7683.	1.6	16
44	Understanding the stability concerns and electronic structure of CsYbX3 (X=Cl,Br) halidoperovskites for optoelectronic applications. Journal of Alloys and Compounds, 2021, 867, 158966.	2.8	16
45	Assessment of dispersionâ€improved exchangeâ€correlation functionals for the simulation of CO₂ binding by alcoholamines. International Journal of Quantum Chemistry, 2014, 114, 805-812.	1.0	14
46	TAO-DFT Study on the Electronic Properties of Diamond-Shaped Graphene Nanoflakes. Nanomaterials, 2020, 10, 1236.	1.9	14
47	Electronic Properties of Linear and Cyclic Boron Nanoribbons from Thermally-Assisted-Occupation Density Functional Theory. Scientific Reports, 2019, 9, 12139.	1.6	13
48	The quantified NTO analysis for the electronic excitations of molecular many-body systems. Chemical Physics Letters, 2011, 514, 362-367.	1.2	11
49	Impact of nonâ€empirically tuning the rangeâ€separation parameter of longâ€range corrected hybrid functionals on ionization potentials, electron affinities, and fundamental gaps. Journal of Computational Chemistry, 2018, 39, 2378-2384.	1.5	11
50	Electronic Properties of Carbon Nanobelts Predicted by Thermally-Assisted-Occupation DFT. Nanomaterials, 2021, 11, 2224.	1.9	11
51	Asymptotic correction schemes for semilocal exchange-correlation functionals. Physical Review A, 2013, 87, .	1.0	10
52	Electronic and Optical Properties of the Narrowest Armchair Graphene Nanoribbons Studied by Density Functional Methods. Australian Journal of Chemistry, 2016, 69, 960.	0.5	10
53	Excitation energies from thermally assisted-occupation density functional theory: Theory and computational implementation. Journal of Chemical Physics, 2020, 153, 084120.	1.2	10
54	The exchange energy of a uniform electron gas experiencing a new, flexible range separation. Chemical Physics Letters, 2009, 478, 283-286.	1.2	9

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55	Assessment of asymptotically corrected model potentials for charge-transfer-like excitations in oligoacenes. Physical Chemistry Chemical Physics, 2014, 16, 21564-21569.	1.3	8
56	TAO-DFT-Based Ab Initio Molecular Dynamics. Frontiers in Chemistry, 2020, 8, 589432.	1.8	8
57	Significant role of the DNA backbone in mediating the transition origin of electronic excitations of B-DNA â€“ implication from long range corrected TDDFT and quantified NTO analysis. Physical Chemistry Chemical Physics, 2012, 14, 9092.	1.3	7
58	The van der Waals interactions in rare-gas dimers: the role of interparticle interactions. Physical Chemistry Chemical Physics, 2016, 18, 3011-3022.	1.3	7
59	TAO-DFT fictitious temperature made simple. RSC Advances, 2022, 12, 12193-12210.	1.7	7
60	Combining density-based dynamical correlation with a reduced-density-matrix strong-correlation description. Physical Review A, 2020, 102, .	1.0	5
61	Simple model for the variation of superfluid density with Zn concentration in YBa2Cu3O7â^'Î´. Physica C: Superconductivity and Its Applications, 2001, 366, 13-22.	0.6	4
62	Assessment of the LFAs-PBE exchangeâ€“correlation potential for high-order harmonic generation of aligned H2+ molecules. RSC Advances, 2016, 6, 33318-33325.	1.7	3
63	Approximate density matrix functionals applied to hetero-atomic bond dissociation. European Physical Journal B, 2020, 93, 1.	0.6	2