

Jeng-Da Chai

List of Publications by Year in descending order

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63
papers

19,415
citations

147801

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63
all docs

63
docs citations

63
times ranked

17789
citing authors

#	ARTICLE	IF	CITATIONS
1	TAO-DFT fictitious temperature made simple. RSC Advances, 2022, 12, 12193-12210.	3.6	7
2	Strain engineering of electronic structure, phonon, and thermoelectric properties of p-type half-Heusler semiconductor. Journal of Alloys and Compounds, 2021, 850, 156615.	5.5	51
3	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.	4.9	22
4	Understanding the stability concerns and electronic structure of CsYbX ₃ (X=Cl,Br) halidoperovskites for optoelectronic applications. Journal of Alloys and Compounds, 2021, 867, 158966.	5.5	16
5	Growth and characterization of crystalline BaSnO ₃ perovskite nanostructures and the influence of heavy Mn doping on its properties. Journal of Alloys and Compounds, 2021, 867, 158900.	5.5	17
6	Origin of pseudo gap and thermoelectric signatures of semimetallic Ru ₂ TaGa: Structural stability from phonon dynamics, mechanical, and thermodynamic predictions. Journal of Physics and Chemistry of Solids, 2021, 154, 110098.	4.0	28
7	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
8	Electronic Properties of Carbon Nanobelts Predicted by Thermally-Assisted-Occupation DFT. Nanomaterials, 2021, 11, 2224.	4.1	11
9	TAO-DFT-Based Ab Initio Molecular Dynamics. Frontiers in Chemistry, 2020, 8, 589432.	3.6	8
10	TAO-DFT investigation of electronic properties of linear and cyclic carbon chains. Scientific Reports, 2020, 10, 13133.	3.3	26
11	Combining density-based dynamical correlation with a reduced-density-matrix strong-correlation description. Physical Review A, 2020, 102, .	2.5	5
12	Excitation energies from thermally assisted-occupation density functional theory: Theory and computational implementation. Journal of Chemical Physics, 2020, 153, 084120.	3.0	10
13	TAO-DFT Study on the Electronic Properties of Diamond-Shaped Graphene Nanoflakes. Nanomaterials, 2020, 10, 1236.	4.1	14
14	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.	2.3	36
15	Thermoelectric properties, phonon, and mechanical stability of new half-metallic quaternary Heusler alloys: FeRhCrZ' (Z=Si and Ge). Journal of Applied Physics, 2020, 127, .	2.5	90
16	Approximate density matrix functionals applied to hetero-atomic bond dissociation. European Physical Journal B, 2020, 93, 1.	1.5	2
17	Electronic Properties of Linear and Cyclic Boron Nanoribbons from Thermally-Assisted-Occupation Density Functional Theory. Scientific Reports, 2019, 9, 12139.	3.3	13
18	Electronic Properties of Triangle-Shaped Graphene Nanoflakes from TAO-DFT. ACS Omega, 2019, 4, 14202-14210.	3.5	18

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19	Novel half-metallic L21 structured full-Heusler compound for promising spintronic applications: A DFT-based computer simulation. <i>Journal of Magnetism and Magnetic Materials</i> , 2019, 487, 165289.	2.3	43
20	Local Density Approximation for the Short-Range Exchange Free Energy Functional. <i>ACS Omega</i> , 2019, 4, 7675-7683.	3.5	16
21	Electronic Properties of MÃ¶bius Cyclacenes Studied by Thermally-Assisted-Occupation Density Functional Theory. <i>Scientific Reports</i> , 2019, 9, 2907.	3.3	23
22	Electronic properties of the coronene series from thermally-assisted-occupation density functional theory. <i>RSC Advances</i> , 2018, 8, 34350-34358.	3.6	21
23	Impact of non-empirically tuning the range-separation parameter of long-range corrected hybrid functionals on ionization potentials, electron affinities, and fundamental gaps. <i>Journal of Computational Chemistry</i> , 2018, 39, 2378-2384.	3.3	11
24	Electronic and Hydrogen Storage Properties of Li-Terminated Linear Boron Chains Studied by TAO-DFT. <i>Scientific Reports</i> , 2018, 8, 13538.	3.3	32
25	Role of exact exchange in thermally-assisted-occupation density functional theory: A proposal of new hybrid schemes. <i>Journal of Chemical Physics</i> , 2017, 146, 044102.	3.0	38
26	Self-consistent determination of the fictitious temperature in thermally-assisted-occupation density functional theory. <i>RSC Advances</i> , 2017, 7, 50496-50507.	3.6	33
27	Effect of Li Termination on the Electronic and Hydrogen Storage Properties of Linear Carbon Chains: A TAO-DFT Study. <i>Scientific Reports</i> , 2017, 7, 4966.	3.3	27
28	Electronic Properties of Cyclacenes from TAO-DFT. <i>Scientific Reports</i> , 2016, 6, 37249.	3.3	50
29	SCAN-based hybrid and double-hybrid density functionals from models without fitted parameters. <i>Journal of Chemical Physics</i> , 2016, 144, 044114.	3.0	126
30	Short- and long-range corrected hybrid density functionals with the D3 dispersion corrections. <i>Journal of Chemical Physics</i> , 2016, 145, 204101.	3.0	26
31	Electronic and Optical Properties of the Narrowest Armchair Graphene Nanoribbons Studied by Density Functional Methods. <i>Australian Journal of Chemistry</i> , 2016, 69, 960.	0.9	10
32	Assessment of the LFAs-PBE exchange-correlation potential for high-order harmonic generation of aligned H2+ molecules. <i>RSC Advances</i> , 2016, 6, 33318-33325.	3.6	3
33	Effect of Li Adsorption on the Electronic and Hydrogen Storage Properties of Acenes: A Dispersion-Corrected TAO-DFT Study. <i>Scientific Reports</i> , 2016, 6, 33081.	3.3	46
34	Role of KekulÃ© and Non-KekulÃ© Structures in the Radical Character of Alternant Polycyclic Aromatic Hydrocarbons: A TAO-DFT Study. <i>Scientific Reports</i> , 2016, 6, 30562.	3.3	63
35	The van der Waals interactions in rare-gas dimers: the role of interparticle interactions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 3011-3022.	2.8	7
36	Assessment of density functional methods for exciton binding energies and related optoelectronic properties. <i>RSC Advances</i> , 2015, 5, 101370-101376.	3.6	47

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37	Electronic Properties of Zigzag Graphene Nanoribbons Studied by TAO-DFT. Journal of Chemical Theory and Computation, 2015, 11, 2003-2011.	5.3	69
38	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
39	Thermally-assisted-occupation density functional theory with generalized-gradient approximations. Journal of Chemical Physics, 2014, 140, 18A521.	3.0	64
40	Assessment of asymptotically corrected model potentials for charge-transfer-like excitations in oligoacenes. Physical Chemistry Chemical Physics, 2014, 16, 21564-21569.	2.8	8
41	Assessment of dispersion-improved exchange-correlation functionals for the simulation of CO ₂ binding by alcoholamines. International Journal of Quantum Chemistry, 2014, 114, 805-812.	2.0	14
42	Restoration of the Derivative Discontinuity in Kohn-Sham Density Functional Theory: An Efficient Scheme for Energy Gap Correction. Physical Review Letters, 2013, 110, 033002.	7.8	46
43	Impact of Metal and Anion Substitutions on the Hydrogen Storage Properties of M-BTT Metal-Organic Frameworks. Journal of the American Chemical Society, 2013, 135, 1083-1091.	13.7	139
44	Long-Range Corrected Hybrid Density Functionals with Improved Dispersion Corrections. Journal of Chemical Theory and Computation, 2013, 9, 263-272.	5.3	535
45	Assessment of density functional methods with correct asymptotic behavior. Physical Chemistry Chemical Physics, 2013, 15, 8352.	2.8	49
46	Asymptotic correction schemes for semilocal exchange-correlation functionals. Physical Review A, 2013, 87, .	2.5	10
47	Long-range corrected hybrid meta-generalized-gradient approximations with dispersion corrections. Journal of Chemical Physics, 2012, 136, 154109.	3.0	101
48	Significant role of the DNA backbone in mediating the transition origin of electronic excitations of B-DNA - implication from long range corrected TDDFT and quantified NTO analysis. Physical Chemistry Chemical Physics, 2012, 14, 9092.	2.8	7
49	Assessment of density functional approximations for the hemibonded structure of the water dimer radical cation. Physical Chemistry Chemical Physics, 2012, 14, 10705.	2.8	41
50	Density functional theory with fractional orbital occupations. Journal of Chemical Physics, 2012, 136, 154104.	3.0	127
51	Seeking for reliable double-hybrid density functionals without fitting parameters: The PBE0-2 functional. Chemical Physics Letters, 2012, 538, 121-125.	2.6	118
52	The quantified NTO analysis for the electronic excitations of molecular many-body systems. Chemical Physics Letters, 2011, 514, 362-367.	2.6	11
53	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.	2.6	17
54	The exchange energy of a uniform electron gas experiencing a new, flexible range separation. Chemical Physics Letters, 2009, 478, 283-286.	2.6	9

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55	Long-range corrected double-hybrid density functionals. <i>Journal of Chemical Physics</i> , 2009, 131, 174105.	3.0	327
56	Optimal operators for Hartree-Fock exchange from long-range corrected hybrid density functionals. <i>Chemical Physics Letters</i> , 2008, 467, 176-178.	2.6	68
57	Long-range corrected hybrid density functionals with damped atom-atom dispersion corrections. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 6615.	2.8	10,464
58	Systematic optimization of long-range corrected hybrid density functionals. <i>Journal of Chemical Physics</i> , 2008, 128, 084106.	3.0	2,890
59	Semiempirical Double-Hybrid Density Functional with Improved Description of Long-Range Correlation. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2702-2712.	2.5	123
60	Orbital-free density functional theory: Kinetic potentials and ab initio local pseudopotentials. <i>Physical Review B</i> , 2007, 75, .	3.2	38
61	Modified Statistical Treatment of Kinetic Energy in the Thomas-Fermi Model. <i>Journal of Physical Chemistry B</i> , 2004, 108, 6870-6876.	2.6	24
62	Dynamic structure factor of liquid and amorphous Ge from ab initio simulations. <i>Physical Review B</i> , 2003, 67, .	3.2	37
63	Simple model for the variation of superfluid density with Zn concentration in $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$. <i>Physica C: Superconductivity and Its Applications</i> , 2001, 366, 13-22.	1.2	4