

Jeng-Da Chai

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

63

papers

14,361

citations

27

h-index

63

g-index

63

ext. papers

16,931

ext. citations

3.9

avg, IF

7.19

L-index

#	Paper	IF	Citations
63	TAO-DFT fictitious temperature made simple.. <i>RSC Advances</i> , 2022 , 12, 12193-12210	3.7	0
62	Synthesis, characterization, antimicrobial, BSA binding, DFT calculation, molecular docking and cytotoxicity of Ni(II) complexes with Schiff base ligands. <i>Journal of Molecular Liquids</i> , 2021 , 328, 115457	6	8
61	Understanding the stability concerns and electronic structure of CsYbX ₃ (X=Cl,Br) halidoperovskites for optoelectronic applications. <i>Journal of Alloys and Compounds</i> , 2021 , 867, 158966	5.7	6
60	Growth and characterization of crystalline BaSnO ₃ perovskite nanostructures and the influence of heavy Mn doping on its properties. <i>Journal of Alloys and Compounds</i> , 2021 , 867, 158900	5.7	6
59	Strain engineering of electronic structure, phonon, and thermoelectric properties of p-type half-Heusler semiconductor. <i>Journal of Alloys and Compounds</i> , 2021 , 850, 156615	5.7	16
58	Origin of pseudo gap and thermoelectric signatures of semimetallic Ru ₂ TaGa: Structural stability from phonon dynamics, mechanical, and thermodynamic predictions. <i>Journal of Physics and Chemistry of Solids</i> , 2021 , 154, 110098	3.9	9
57	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021 , 155, 084801	3.9	115
56	Electronic Properties of Carbon Nanobelts Predicted by Thermally-Assisted-Occupation DFT. <i>Nanomaterials</i> , 2021 , 11,	5.4	3
55	TAO-DFT Study on the Electronic Properties of Diamond-Shaped Graphene Nanoflakes. <i>Nanomaterials</i> , 2020 , 10,	5.4	7
54	Robust stability, half-metallic ferrimagnetism and thermoelectric properties of new quaternary Heusler material: A first principles approach. <i>Journal of Magnetism and Magnetic Materials</i> , 2020 , 502, 166562	2.8	23
53	Approximate density matrix functionals applied to hetero-atomic bond dissociation. <i>European Physical Journal B</i> , 2020 , 93, 1	1.2	1
52	TAO-DFT-Based Molecular Dynamics. <i>Frontiers in Chemistry</i> , 2020 , 8, 589432	5	3
51	TAO-DFT investigation of electronic properties of linear and cyclic carbon chains. <i>Scientific Reports</i> , 2020 , 10, 13133	4.9	12
50	Combining density-based dynamical correlation with a reduced-density-matrix strong-correlation description. <i>Physical Review A</i> , 2020 , 102,	2.6	2
49	Excitation energies from thermally assisted-occupation density functional theory: Theory and computational implementation. <i>Journal of Chemical Physics</i> , 2020 , 153, 084120	3.9	4
48	Thermoelectric properties, phonon, and mechanical stability of new half-metallic quaternary Heusler alloys: FeRhCrZ (Z = Si and Ge). <i>Journal of Applied Physics</i> , 2020 , 127, 165102	2.5	42
47	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	2.8	28

46	Local Density Approximation for the Short-Range Exchange Free Energy Functional. <i>ACS Omega</i> , 2019 , 4, 7675-7683	3.9	9
45	Electronic Properties of Möbius Cyclacenes Studied by Thermally-Assisted-Occupation Density Functional Theory. <i>Scientific Reports</i> , 2019 , 9, 2907	4.9	17
44	Electronic Properties of Linear and Cyclic Boron Nanoribbons from Thermally-Assisted-Occupation Density Functional Theory. <i>Scientific Reports</i> , 2019 , 9, 12139	4.9	8
43	Electronic Properties of Triangle-Shaped Graphene Nanoflakes from TAO-DFT. <i>ACS Omega</i> , 2019 , 4, 14262-14270	4.9	10
42	Electronic properties of the coronene series from thermally-assisted-occupation density functional theory.. <i>RSC Advances</i> , 2018 , 8, 34350-34358	3.7	14
41	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	3.5	8
40	Electronic and Hydrogen Storage Properties of Li-Terminated Linear Boron Chains Studied by TAO-DFT. <i>Scientific Reports</i> , 2018 , 8, 13538	4.9	25
39	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	3.9	27
38	Self-consistent determination of the fictitious temperature in thermally-assisted-occupation density functional theory. <i>RSC Advances</i> , 2017 , 7, 50496-50507	3.7	25
37	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	4.9	23
36	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	4.9	32
35	Role of Kekulé and Non-Kekulé Structures in the Radical Character of Alternant Polycyclic Aromatic Hydrocarbons: A TAO-DFT Study. <i>Scientific Reports</i> , 2016 , 6, 30562	4.9	46
34	The van der Waals interactions in rare-gas dimers: the role of interparticle interactions. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 3011-22	3.6	5
33	Electronic Properties of Cyclacenes from TAO-DFT. <i>Scientific Reports</i> , 2016 , 6, 37249	4.9	37
32	SCAN-based hybrid and double-hybrid density functionals from models without fitted parameters. <i>Journal of Chemical Physics</i> , 2016 , 144, 044114	3.9	97
31	Short- and long-range corrected hybrid density functionals with the D3 dispersion corrections. <i>Journal of Chemical Physics</i> , 2016 , 145, 204101	3.9	21
30	Electronic and Optical Properties of the Narrowest Armchair Graphene Nanoribbons Studied by Density Functional Methods. <i>Australian Journal of Chemistry</i> , 2016 , 69, 960	1.2	7
29	Assessment of the LFAs-PBE exchange-correlation potential for high-order harmonic generation of aligned H ₂ ⁺ molecules. <i>RSC Advances</i> , 2016 , 6, 33318-33325	3.7	2

28	Electronic Properties of Zigzag Graphene Nanoribbons Studied by TAO-DFT. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 2003-11	6.4	56
27	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015 , 113, 184-215	1.7	2068
26	Assessment of density functional methods for exciton binding energies and related optoelectronic properties. <i>RSC Advances</i> , 2015 , 5, 101370-101376	3.7	36
25	Thermally-assisted-occupation density functional theory with generalized-gradient approximations. <i>Journal of Chemical Physics</i> , 2014 , 140, 18A521	3.9	49
24	Assessment of asymptotically corrected model potentials for charge-transfer-like excitations in oligoacenes. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 21564-9	3.6	8
23	Assessment of dispersion-improved exchange-correlation functionals for the simulation of CO ₂ binding by alcoholamines. <i>International Journal of Quantum Chemistry</i> , 2014 , 114, 805-812	2.1	10
22	Restoration of the derivative discontinuity in Kohn-Sham density functional theory: an efficient scheme for energy gap correction. <i>Physical Review Letters</i> , 2013 , 110, 033002	7.4	44
21	Impact of metal and anion substitutions on the hydrogen storage properties of M-BTT metal-organic frameworks. <i>Journal of the American Chemical Society</i> , 2013 , 135, 1083-91	16.4	128
20	Long-Range Corrected Hybrid Density Functionals with Improved Dispersion Corrections. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 263-72	6.4	321
19	Assessment of density functional methods with correct asymptotic behavior. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 8352-61	3.6	44
18	Asymptotic correction schemes for semilocal exchange-correlation functionals. <i>Physical Review A</i> , 2013 , 87,	2.6	10
17	Seeking for reliable double-hybrid density functionals without fitting parameters: The PBE0-2 functional. <i>Chemical Physics Letters</i> , 2012 , 538, 121-125	2.5	92
16	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. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 9092-103	3.6	5
15	Assessment of density functional approximations for the hemibonded structure of the water dimer radical cation. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 10705-12	3.6	38
14	Density functional theory with fractional orbital occupations. <i>Journal of Chemical Physics</i> , 2012 , 136, 154104	3.9	99
13	Long-range corrected hybrid meta-generalized-gradient approximations with dispersion corrections. <i>Journal of Chemical Physics</i> , 2012 , 136, 154109	3.9	88
12	The quantified NTO analysis for the electronic excitations of molecular many-body systems. <i>Chemical Physics Letters</i> , 2011 , 514, 362-367	2.5	9
11	Orbital-free density functional theory: Linear scaling methods for kinetic potentials, and applications to solid Al and Si. <i>Chemical Physics Letters</i> , 2009 , 473, 263-267	2.5	12

10	The exchange energy of a uniform electron gas experiencing a new, flexible range separation. <i>Chemical Physics Letters</i> , 2009 , 478, 283-286	2.5	9
9	Long-range corrected double-hybrid density functionals. <i>Journal of Chemical Physics</i> , 2009 , 131, 174105	3.9	271
8	Systematic optimization of long-range corrected hybrid density functionals. <i>Journal of Chemical Physics</i> , 2008 , 128, 084106	3.9	2290
7	Semiempirical double-hybrid density functional with improved description of long-range correlation. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 2702-12	2.8	114
6	Optimal operators for Hartree-Fock exchange from long-range corrected hybrid density functionals. <i>Chemical Physics Letters</i> , 2008 , 467, 176-178	2.5	61
5	Long-range corrected hybrid density functionals with damped atom-atom dispersion corrections. <i>Physical Chemistry Chemical Physics</i> , 2008 , 10, 6615-20	3.6	7709
4	Orbital-free density functional theory: Kinetic potentials and ab initio local pseudopotentials. <i>Physical Review B</i> , 2007 , 75,	3.3	32
3	Modified Statistical Treatment of Kinetic Energy in the Thomas-Fermi Model. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 6870-6876	3.4	21
2	Dynamic structure factor of liquid and amorphous Ge from ab initio simulations. <i>Physical Review B</i> , 2003 , 67,	3.3	33
1	Simple model for the variation of superfluid density with Zn concentration in YBa ₂ Cu ₃ O _{7-δ} . <i>Physica C: Superconductivity and Its Applications</i> , 2001 , 366, 13-22	1.3	4