Jeng-Da Chai

List of Publications by Citations

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	Long-range corrected hybrid density functionals with damped atom-atom dispersion corrections. *Physical Chemistry Chemical Physics*, **2008**, 10, 6615-20	3.6	7709
62	Systematic optimization of long-range corrected hybrid density functionals. *Journal of Chemical Physics*, **2008**, 128, 084106	3.9	2290
61	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
60	Long-Range Corrected Hybrid Density Functionals with Improved Dispersion Corrections. *Journal of Chemical Theory and Computation*, **2013**, 9, 263-72	6.4	321
59	Long-range corrected double-hybrid density functionals. *Journal of Chemical Physics*, **2009**, 131, 174105	3.9	271
58	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, 1083-91	16.4	128
57	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
56	Semiempirical double-hybrid density functional with improved description of long-range correlation. *Journal of Physical Chemistry A*, **2008**, 112, 2702-12	2.8	114
55	Density functional theory with fractional orbital occupations. *Journal of Chemical Physics*, **2012**, 136, 154104	3.9	99
54	SCAN-based hybrid and double-hybrid density functionals from models without fitted parameters. *Journal of Chemical Physics*, **2016**, 144, 044114	3.9	97
53	Seeking for reliable double-hybrid density functionals without fitting parameters: The PBE0-2 functional. *Chemical Physics Letters*, **2012**, 538, 121-125	2.5	92
52	Long-range corrected hybrid meta-generalized-gradient approximations with dispersion corrections. *Journal of Chemical Physics*, **2012**, 136, 154109	3.9	88
51	Optimal operators for Hartree–Fock exchange from long-range corrected hybrid density functionals. *Chemical Physics Letters*, **2008**, 467, 176-178	2.5	61
50	Electronic Properties of Zigzag Graphene Nanoribbons Studied by TAO-DFT. *Journal of Chemical Theory and Computation*, **2015**, 11, 2003-11	6.4	56
49	Thermally-assisted-occupation density functional theory with generalized-gradient approximations. *Journal of Chemical Physics*, **2014**, 140, 18A521	3.9	49
48	Role of Kekulé and Non-Kekulé Structures in the Radical Character of Alternant Polycyclic Aromatic Hydrocarbons: A TAO-DFT Study. *Scientific Reports*, **2016**, 6, 30562	4.9	46
47	Restoration of the derivative discontinuity in Kohn-Sham density functional theory: an efficient scheme for energy gap correction. *Physical Review Letters*, **2013**, 110, 033002	7.4	44

46	Assessment of density functional methods with correct asymptotic behavior. *Physical Chemistry Chemical Physics*, **2013**, 15, 8352-61	3.6	44
45	Thermoelectric properties, phonon, and mechanical stability of new half-metallic quaternary Heusler alloys: FeRhCrZ (Z = Si and Ge). *Journal of Applied Physics*, **2020**, 127, 165102	2.5	42
44	Assessment of density functional approximations for the hemibonded structure of the water dimer radical cation. *Physical Chemistry Chemical Physics*, **2012**, 14, 10705-12	3.6	38
43	Electronic Properties of Cyclacenes from TAO-DFT. *Scientific Reports*, **2016**, 6, 37249	4.9	37
42	Assessment of density functional methods for exciton binding energies and related optoelectronic properties. *RSC Advances*, **2015**, 5, 101370-101376	3.7	36
41	Dynamic structure factor of liquid and amorphous Ge from ab initio simulations. *Physical Review B*, **2003**, 67,	3.3	33
40	Effect of Li Adsorption on the Electronic and Hydrogen Storage Properties of Acenes: A Dispersion-Corrected TAO-DFT Study. *Scientific Reports*, **2016**, 6, 33081	4.9	32
39	Orbital-free density functional theory: Kinetic potentials and ab initio local pseudopotentials. *Physical Review B*, **2007**, 75,	3.3	32
38	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	2.8	28
37	Role of exact exchange in thermally-assisted-occupation density functional theory: A proposal of new hybrid schemes. *Journal of Chemical Physics*, **2017**, 146, 044102	3.9	27
36	Self-consistent determination of the fictitious temperature in thermally-assisted-occupation density functional theory. *RSC Advances*, **2017**, 7, 50496-50507	3.7	25
35	Electronic and Hydrogen Storage Properties of Li-Terminated Linear Boron Chains Studied by TAO-DFT. *Scientific Reports*, **2018**, 8, 13538	4.9	25
34	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	2.8	23
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	4.9	23
32	Modified Statistical Treatment of Kinetic Energy in the Thomas–Fermi Model. *Journal of Physical Chemistry B*, **2004**, 108, 6870-6876	3.4	21
31	Short- and long-range corrected hybrid density functionals with the D3 dispersion corrections. *Journal of Chemical Physics*, **2016**, 145, 204101	3.9	21
30	Electronic Properties of Möbius Cyclacenes Studied by Thermally-Assisted-Occupation Density Functional Theory. *Scientific Reports*, **2019**, 9, 2907	4.9	17
29	Strain engineering of electronic structure, phonon, and thermoelectric properties of p-type half-Heusler semiconductor. *Journal of Alloys and Compounds*, **2021**, 850, 156615	5.7	16

28	Electronic properties of the coronene series from thermally-assisted-occupation density functional theory.. *RSC Advances*, **2018**, 8, 34350-34358	3.7	14
27	Electronic Properties of Triangle-Shaped Graphene Nanoflakes from TAO-DFT. *ACS Omega*, **2019**, 4, 14202-14210	3.7	12
26	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	2.5	12
25	TAO-DFT investigation of electronic properties of linear and cyclic carbon chains. *Scientific Reports*, **2020**, 10, 13133	4.9	12
24	Assessment of dispersion-improved exchange-correlation functionals for the simulation of CO2 binding by alcoholamines. *International Journal of Quantum Chemistry*, **2014**, 114, 805-812	2.1	10
23	Asymptotic correction schemes for semilocal exchange-correlation functionals. *Physical Review A*, **2013**, 87,	2.6	10
22	Local Density Approximation for the Short-Range Exchange Free Energy Functional. *ACS Omega*, **2019**, 4, 7675-7683	3.9	9
21	The quantified NTO analysis for the electronic excitations of molecular many-body systems. *Chemical Physics Letters*, **2011**, 514, 362-367	2.5	9
20	The exchange energy of a uniform electron gas experiencing a new, flexible range separation. *Chemical Physics Letters*, **2009**, 478, 283-286	2.5	9
19	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	3.9	9
18	Electronic Properties of Linear and Cyclic Boron Nanoribbons from Thermally-Assisted-Occupation Density Functional Theory. *Scientific Reports*, **2019**, 9, 12139	4.9	8
17	Assessment of asymptotically corrected model potentials for charge-transfer-like excitations in oligoacenes. *Physical Chemistry Chemical Physics*, **2014**, 16, 21564-9	3.6	8
16	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	6	8
15	Impact of non-empirically tuning the range-separation parameter of long-range corrected hybrid functionals on ionization potentials, electron affinities, and fundamental gaps. *Journal of Computational Chemistry*, **2018**, 39, 2378-2384	3.5	8
14	TAO-DFT Study on the Electronic Properties of Diamond-Shaped Graphene Nanoflakes. *Nanomaterials*, **2020**, 10,	5.4	7
13	Electronic and Optical Properties of the Narrowest Armchair Graphene Nanoribbons Studied by Density Functional Methods. *Australian Journal of Chemistry*, **2016**, 69, 960	1.2	7
12	Understanding the stability concerns and electronic structure of CsYbX3 (X=Cl,Br) halidoperovskites for optoelectronic applications. *Journal of Alloys and Compounds*, **2021**, 867, 158966	5.7	6
11	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	5.7	6

List of Publications

10	The van der Waals interactions in rare-gas dimers: the role of interparticle interactions. *Physical Chemistry Chemical Physics*, **2016**, 18, 3011-22	3.6	5
9	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, 9092-103	3.6	5
8	Simple model for the variation of superfluid density with Zn concentration in YBa2Cu3O7 *Physica C: Superconductivity and Its Applications*, **2001**, 366, 13-22	1.3	4
7	Excitation energies from thermally assisted-occupation density functional theory: Theory and computational implementation. *Journal of Chemical Physics*, **2020**, 153, 084120	3.9	4
6	TAO-DFT-Based Molecular Dynamics. *Frontiers in Chemistry*, **2020**, 8, 589432	5	3
5	Electronic Properties of Carbon Nanobelts Predicted by Thermally-Assisted-Occupation DFT. *Nanomaterials*, **2021**, 11,	5.4	3
4	Combining density-based dynamical correlation with a reduced-density-matrix strong-correlation description. *Physical Review A*, **2020**, 102,	2.6	2
3	Assessment of the LFAs-PBE exchange correlation potential for high-order harmonic generation of aligned H2+ molecules. *RSC Advances*, **2016**, 6, 33318-33325	3.7	2
2	Approximate density matrix functionals applied to hetero-atomic bond dissociation. *European Physical Journal B*, **2020**, 93, 1	1.2	1
1	TAO-DFT fictitious temperature made simple.. *RSC Advances*, **2022**, 12, 12193-12210	3.7	0