MichaÅ, Hapka

List of Publications by Year in descending order

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623574 642610 40 618 14 23 citations g-index h-index papers 40 40 40 636 docs citations times ranked citing authors all docs

#	Article	IF	Citations
1	An efficient implementation of time-dependent linear-response theory for strongly orthogonal geminal wave function models. Journal of Chemical Physics, 2022, 156, 174102.	1.2	6
2	Efficient Adiabatic Connection Approach for Strongly Correlated Systems: Application to Singlet–Triplet Gaps of Biradicals. Journal of Physical Chemistry Letters, 2022, 13, 4570-4578.	2.1	11
3	Dispersion Interactions in Exciton-Localized States. Theory and Applications to π–π* and nâ^'Ï€* Excited States. Journal of Chemical Theory and Computation, 2022, 18, 3497-3511.	2.3	4
4	Dataset of noncovalent intermolecular interaction energy curves for 24 small high-spin open-shell dimers. Journal of Chemical Physics, 2021, 154, 134106.	1.2	5
5	In pursuit of universality. Nature Reviews Chemistry, 2021, 5, 520-521.	13.8	1
6	Symmetry-Adapted Perturbation Theory Based on Multiconfigurational Wave Function Description of Monomers. Journal of Chemical Theory and Computation, 2021, 17, 5538-5555.	2.3	18
7	Density Matrix Renormalization Group with Dynamical Correlation via Adiabatic Connection. Journal of Chemical Theory and Computation, 2021, 17, 7575-7585.	2.3	26
8	The effect of weak intermolecular interactions on the nuclear magnetic resonance shielding constant in N ₂ . Magnetic Resonance in Chemistry, 2020, 58, 245-248.	1.1	2
9	How Much Dispersion Energy Is Included in the Multiconfigurational Interaction Energy?. Journal of Chemical Theory and Computation, 2020, 16, 6280-6293.	2.3	8
10	Reduced Density Matrix-Driven Complete Active Apace Self-Consistent Field Corrected for Dynamic Correlation from the Adiabatic Connection. Journal of Chemical Theory and Computation, 2020, 16, 4351-4360.	2.3	11
11	Long-range-corrected multiconfiguration density functional with the on-top pair density. Journal of Chemical Physics, 2020, 152, 094102.	1.2	15
12	Molecular multibond dissociation with small complete active space augmented by correlation density functionals. Journal of Chemical Physics, 2020, 152, 204118.	1.2	4
13	Assessment of SAPT(DFT) with meta-GGA functionals. Journal of Molecular Modeling, 2020, 26, 102.	0.8	7
14	Local Enhancement of Dynamic Correlation in Excited States: Fresh Perspective on Ionicity and Development of Correlation Density Functional Approximation Based on the On-Top Pair Density. Journal of Physical Chemistry Letters, 2020, 11, 5883-5889.	2.1	10
15	Capturing the Dynamic Correlation for Arbitrary Spin-Symmetry CASSCF Reference with Adiabatic Connection Approaches: Insights into the Electronic Structure of the Tetramethyleneethane Diradical. Journal of Physical Chemistry Letters, 2019, 10, 4668-4674.	2.1	16
16	On the Nature of Luminescence Thermochromism of Multinuclear Copper(I) Benzoate Complexes in the Crystalline State. Crystals, 2019, 9, 36.	1.0	8
17	Toward Heterolytic Bond Dissociation of Dihydrogen: The Study of Hydrogen in Arsenolite under High Pressure. Journal of Physical Chemistry C, 2019, 123, 16868-16872.	1.5	6
18	Second-Order Exchange-Dispersion Energy Based on a Multireference Description of Monomers. Journal of Chemical Theory and Computation, 2019, 15, 6712-6723.	2.3	11

#	Article	IF	CITATIONS
19	Second-Order Dispersion Energy Based on Multireference Description of Monomers. Journal of Chemical Theory and Computation, 2019, 15, 1016-1027.	2.3	17
20	How and Why Does Helium Permeate Nonporous Arsenolite Under High Pressure?. ChemPhysChem, 2018, 19, 857-864.	1.0	10
21	Intricacies of van der Waals Interactions in Systems with Elongated Bonds Revealed by Electron-Groups Embedding and High-Level Coupled-Cluster Approaches. Journal of Chemical Theory and Computation, 2017, 13, 5404-5419.	2.3	16
22	The nature of three-body interactions in DFT: Exchange and polarization effects. Journal of Chemical Physics, 2017, 147, 084106.	1.2	15
23	Theoretical study of the buffer-gas cooling and trapping of $CrH(X6\hat{1}_{\pm}+)$ by 3He atoms. Journal of Chemical Physics, 2016, 145, 214305.	1.2	4
24	Experimental and Theoretical Studies of Low-Energy Penning Ionization of NH3, CH3F, and CHF3. ChemPhysChem, 2016, 17, 3776-3782.	1.0	5
25	Communication: Importance of rotationally inelastic processes in low-energy Penning ionization of CHF3. Journal of Chemical Physics, 2016, 144, 221102.	1.2	10
26	Interaction of Boron–Nitrogen Doped Benzene Isomers with Water. Journal of Physical Chemistry A, 2016, 120, 6287-6302.	1.1	15
27	Employing Range Separation on the meta-GGA Rung: New Functional Suitable for Both Covalent and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2016, 12, 3662-3673.	2.3	10
28	Noncovalent interactions determine the conformation of aurophilic complexes with 2-mercapto-4-methyl-5-thiazoleacetic acid ligands. Dalton Transactions, 2015, 44, 13641-13650.	1.6	5
29	Observation of orbiting resonances in He(3S1) + NH3 Penning ionization. Journal of Chemical Physics, 2015, 142, 164305.	1.2	57
30	Dynamics of gas phase Ne* + NH3 and Ne* + ND3 Penning ionisation at low temperatures. Journal of Chemical Physics, 2014, 140, 244302.	1.2	82
31	Tuned range-separated hybrid functionals in the symmetry-adapted perturbation theory. Journal of Chemical Physics, 2014, 141, 134120.	1.2	18
32	Density functional theory approach to gold-ligand interactions: Separating true effects from artifacts. Journal of Chemical Physics, 2014, 140, 244313.	1.2	14
33	Theoretical Studies of Potential Energy Surface and Bound States of the Strongly Bound He(¹ S)–BeO (¹ Σ ⁺) Complex. Journal of Physical Chemistry A, 2013, 117, 6657-6663.	1.1	15
34	First-principle interaction potentials for metastable He(3S) and Ne(3P) with closed-shell molecules: Application to Penning-ionizing systems. Journal of Chemical Physics, 2013, 139, 014307.	1.2	18
35	Symmetry-adapted perturbation theory based on unrestricted Kohn-Sham orbitals for high-spin open-shell van der Waals complexes. Journal of Chemical Physics, 2012, 137, 164104.	1.2	42
36	Optical absorption spectra of gold clusters Aun (n = 4, 6, 8,12, 20) from long-range corrected functionals with optimal tuning. Journal of Chemical Physics, 2012, 137, 114302.	1.2	60

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#	Article	lF	CITATION
37	Interactions of ThO(X) with He, Ne and Ar from the ab initio coupled cluster and symmetry adapted perturbation theory calculations. Chemical Physics, 2012, 399, 50-58.	0.9	5
38	A density functional theory approach to noncovalent interactions via interacting monomer densities. Physical Chemistry Chemical Physics, 2010, 12, 14686.	1.3	9
39	Differential action of methylselenocysteine in control and alloxan-diabetic rabbits. Chemico-Biological Interactions, 2009, 177, 161-171.	1.7	13
40	Rangeâ€separated multiconfigurational density functional theory methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 0, , e1566.	6.2	9