Andrew M Sand

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5825238/publications.pdf

Version: 2024-02-01

21	1,063	759233 12	677142 22
papers	citations	h-index	g-index

25	25	25	1363
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
2	Correlated-Participating-Orbitals Pair-Density Functional Method and Application to Multiplet Energy Splittings of Main-Group Divalent Radicals. Journal of Chemical Theory and Computation, 2016, 12, 4274-4283.	5.3	55
3	Synthesis and Photophysics of Benzotexaphyrin: A Near-Infrared Emitter and Photosensitizer. Journal of the American Chemical Society, 2008, 130, 15782-15783.	13.7	43
4	Analytic Gradients for Complete Active Space Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2018, 14, 126-138.	5.3	40
5	Strongly correlated barriers to rotation from parametric two-electron reduced-density-matrix methods in application to the isomerization of diazene. Journal of Chemical Physics, 2012, 136, 034112.	3.0	31
6	Synthesis and characterization of WS2 nanotube supported cobalt catalyst for hydrodesulfurization. Materials Research Bulletin, 2012, 47, 1653-1660.	5.2	31
7	Efficient algorithm for multiconfiguration pair-density functional theory with application to the heterolytic dissociation energy of ferrocene. Journal of Chemical Physics, 2017, 146, 034101.	3.0	29
8	State-interaction pair-density functional theory. Journal of Chemical Physics, 2018, 149, 024106.	3.0	27
9	Possible effect of carbon nanotube diameter on gasâ€“surface interactions â€“ The case of benzene, water, and n-pentane adsorption on SWCNTs at ultra-high vacuum conditions. Chemical Physics Letters, 2009, 476, 227-231.	2.6	26
10	Adsorption of Thiophene on Inorganic MoS2 Fullerene-Like Nanoparticles. Catalysis Letters, 2009, 129, 66-70.	2.6	17
11	Enhanced computational efficiency in the direct determination of the two-electron reduced density matrix from the anti-Hermitian contracted SchrÃ¶dinger equation with application to ground and excited states of conjugated Ï€-systems. Journal of Chemical Physics, 2015, 143, 134110.	3.0	17
12	Analytic gradients for state-averaged multiconfiguration pair-density functional theory. Journal of Chemical Physics, 2020, 153, 014106.	3.0	16
13	Calculation of Chemical Reaction Barrier Heights by Multiconfiguration Pair-Density Functional Theory with Correlated Participating Orbitals. Journal of Physical Chemistry A, 2019, 123, 9809-9817.	2.5	11
14	Adsorption kinetics of methanol in carbon nanotubes revisited â€“ solvent effects and pitfalls in ultra-high vacuum surface science experiments. Chemical Physics Letters, 2009, 473, 131-134.	2.6	10
15	Adsorption and reaction kinetics of small organic molecules on WS2 nanotubes: An ultra-high vacuum study. Chemical Physics Letters, 2009, 479, 109-112.	2.6	9
16	Effect of molecular-orbital rotations on ground-state energies in the parametric two-electron reduced density matrix method. Journal of Chemical Physics, 2013, 138, 244102.	3.0	8
17	Analytic gradients for multiconfiguration pair-density functional theory with density fitting: Development and application to geometry optimization in the ground and excited states. Journal of Chemical Physics, 2021, 154, 074108.	3.0	8
18	Parametric two-electron reduced-density-matrix method with application to diradical rectangular H4. Computational and Theoretical Chemistry, 2013, 1003, 44-49.	2.5	7

#	Article	IF	Citations
19	Adsorption kinetics of small organic molecules on thick and thinner layers of carbon nanotubes. Chemical Physics Letters, 2009, 470, 300-303.	2.6	5
20	Modulating the Electronic Structure of Chromophores by Chemical Substituents for Efficient Energy Transfer: Application to Fluorone. Journal of Physical Chemistry A, 2014, 118, 6085-6091.	2.5	4
21	A multiconfiguration pair-density functional theory-based approach to molecular junctions. Journal of Chemical Physics, 2021, 155, 114115.	3.0	2