Andrew M Sand

List of Publications by Year
in descending order

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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	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
2	A multiconfiguration pair-density functional theory-based approach to molecular junctions. Journal of Chemical Physics, 2021, 155, 114115.	3.0	2
3	Analytic gradients for state-averaged multiconfiguration pair-density functional theory. Journal of Chemical Physics, 2020, 153, 014106.	3.0	16
4	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
5	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
6	Analytic Gradients for Complete Active Space Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2018, 14, 126-138.	5.3	40
7	State-interaction pair-density functional theory. Journal of Chemical Physics, 2018, 149, 024106.	3.0	27
8	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
9	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
10	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
11	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
12	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
13	Parametric two-electron reduced-density-matrix method with application to diradical rectangular H4. Computational and Theoretical Chemistry, 2013, 1003, 44-49.	2.5	7
14	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
15	Synthesis and characterization of WS2 nanotube supported cobalt catalyst for hydrodesulfurization. Materials Research Bulletin, 2012, 47, 1653-1660.	5.2	31
16	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
17	Adsorption of Thiophene on Inorganic MoS2 Fullerene-Like Nanoparticles. Catalysis Letters, 2009, 129, 66-70.	2.6	17
18	Adsorption kinetics of small organic molecules on thick and thinner layers of carbon nanotubes. Chemical Physics Letters, 2009, 470, 300-303.	2.6	5

#	Article	IF	Citations
19	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
20	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
21	Synthesis and Photophysics of Benzotexaphyrin: A Near-Infrared Emitter and Photosensitizer. Journal of the American Chemical Society, 2008, 130, 15782-15783.	13.7	43