Martina Kieninger

List of Publications by Year
in descending order

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36	582	567281 15	642732 23
papers	citations	h-index	g-index

43	43	43	447
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Tautomeric Forms of 2-Thiobarbituric Acid As Studied in the Solid, in Polar Solutions, and on Gold Nanoparticles. Journal of Physical Chemistry C, 2007, 111, 3369-3383.	3.1	59
2	The FO2 radical: a new success of density functional theory. Chemical Physics Letters, 1995, 245, 488-497.	2.6	50
3	Density functional studies on hydrogen-bonded complexes. International Journal of Quantum Chemistry, 1994, 52, 465-478.	2.0	46
4	Complete basis set and density functional determination of the enthalpy of formation of the controversial HO3 radical: a discrepancy between theory and experiment. Chemical Physics Letters, 2002, 365, 440-449.	2.6	39
5	Density functional investigations of carboxyl free radicals: Formyloxyl, acetyloxyl, and benzoyloxyl radicals. International Journal of Quantum Chemistry, 1998, 70, 253-267.	2.0	34
6	Density Functional Theory Is More Accurate Than Coupled-Cluster Theory in the Study of the Thermochemistry of Species Containing the Fâˆ’O Bond. Journal of Physical Chemistry A, 1999, 103, 147-151.	2.5	32
7	A discrepancy between experimental and theoretical thermochemical characterization of some oxygen fluorides. Chemical Physics Letters, 1998, 287, 597-600.	2.6	28
8	The chemical Hamiltonian approach in density functional theory. Chemical Physics Letters, 1994, 230, 485-490.	2.6	22
9	Equilibrium structure of the carbon dioxide-water complex in the gas phase: an ab initio and density functional study. Computational and Theoretical Chemistry, 1997, 390, 157-167.	1.5	21
10	Density functional and coupled-cluster calculations of isodesmic reactions involving fluorine oxides. Chemical Physics Letters, 1999, 301, 331-335.	2.6	20
11	Density functional computational thermochemistry: solving the discrepancy between MO and DFT calculations on the enthalpy of formation of sulfine, CH2Ï˜...SÏ˜...O. Chemical Physics Letters, 2002, 355, 207-213.	2.6	19
12	Reinvestigation of the Deceptively Simple Reaction of Toluene with OH and the Fate of the Benzyl Radical: The â€œHiddenâ€•Routes to Cresols and Benzaldehyde. Journal of Physical Chemistry A, 2020, 124, 5917-5930.	2.5	18
13	SVECV â€f12: Benchmark of a composite scheme for accurate and cost effective evaluation of reaction barriers. International Journal of Quantum Chemistry, 2021, 121, e26745.	2.0	18
14	Conformational and energetic properties of the ammonia dimer?comparison of post-Hartree?Fock and density functional methods. Journal of Computational Chemistry, 1996, 17, 1508-1519.	3.3	17
15	Density functional computational thermochemistry: determination of the enthalpy of formation of sulfine, CH2Ï˜...SÏ˜...O, at room temperature. Chemical Physics Letters, 2000, 329, 145-153.	2.6	17
16	Density Functional Computational Thermochemistry:Â Isomerization of Sulfine and Its Enthalpy of Formation. Journal of Physical Chemistry A, 2001, 105, 9912-9916.	2.5	17
17	A New Perspective in the Lewis Acid Catalyzed Ring Opening of Epoxides. Theoretical Study of Some Complexes of Methanol, Acetic Acid, Dimethyl Ether, Diethyl Ether, and Ethylene Oxide with Boron Trifluoride. Journal of Physical Chemistry A, 2006, 110, 11734-11751.	2.5	12
18	Density Functional Computational Thermochemistry:â€‰ Determination of the Enthalpy of Formation of Methanethial-S,S-dioxide (Sulfene). Journal of Physical Chemistry A, 2003, 107, 518-521.	2.5	11

#	Article	IF	Citations
19	Molecular Structure and Internal Rotation in 2,3,5,6-Tetrafluoroanisole as Studied by Gas-Phase Electron Diffraction and Quantum Chemical Calculations. Journal of Physical Chemistry A, 2005, 109, 394-399.	2.5	11
20	Density functional study of isomerization of fluoro- and chloroformaldehyde radical cations. Journal of Computational Chemistry, 1996, 17, 1309-1317.	3.3	10
21	Density functional and ab initio study of the free radical MgNC. Computational and Theoretical Chemistry, 1998, 422, 133-141.	1.5	10
22	Density functional studies of internal rotation: formamide as a prototype of the peptide bond. Journal of Molecular Structure, 1996, 375, 181-188.	3.6	9
23	A comparative density functional study of the torsional potential of 4-fluoro (trifluoromethoxy)benzene and related species. Chemical Physics Letters, 2004, 389, 405-412.	2.6	7
24	Glycine conformations: gradient-corrected DFT-studies. Computational and Theoretical Chemistry, 1998, 433, 193-201.	1.5	6
25	On the structure, infrared and Raman spectra of the 2:1 cysteineâ€“Zn complex. Theoretical Chemistry Accounts, 2010, 125, 279-291.	1.4	6
26	Computational chemistry as an analytical tool: thermochemical examples in atmospheric chemistry. Pure and Applied Chemistry, 1998, 70, 2301-2307.	1.9	5
27	Basis Set Effects in the Description of the Cl-O Bond in ClO and XClO/ClOX Isomers (Xâ€‰=â€‰H, O, and Cl) Using DFT and CCSD(T) Methods. Journal of Chemistry, 2019, 2019, 1-23.	1.9	5
28	A reinvestigation of the deceptively simple reaction of toluene with OH, and the fate of the benzyl radical: a combined thermodynamic and kinetic study on the competition between OH-addition and H-abstraction reactions. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	5
29	Computational determination of the enthalpy of formation of alkylthial S-oxides and alkylthione S-oxides: a study of (Z)-propanethial-S-oxide, the lachrymatory factor of the onion (Allium cepa). Physical Chemistry Chemical Physics, 2002, 4, 4328-4333.	2.8	3
30	Comparison of large basis set DFT and MP2 calculations in the study of the barrier for internal rotation of 2,3,5,6-tetrafluoroanisole. International Journal of Quantum Chemistry, 2007, 107, 403-417.	2.0	3
31	On the experimental structure of monoperoxocarbonic acid and the enthalpy of formation of carbonic acid, peroxyformic acid and monoperoxocarbonic acid in gas phase. Chemical Physics Letters, 2009, 480, 52-56.	2.6	3
32	Enthalpies of formation of the benzyloxyl, benzylperoxyl, hydroxyphenyl radicals and related species on the potential energy surface for the reaction of toluene with the hydroxyl radical. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	3
33	Title is missing!. Molecular Engineering, 1997, 7, 317-348.	0.2	2
34	Using density functional theory to increase the accuracy of experimental crystal structures: The case of potassium peroxocarbonate. Journal of Molecular Structure, 2017, 1146, 1-4.	3.6	1
35	A Festschrift in honor of SÃ¡ndor Suhaiâ€™s 65th birthday. Theoretical Chemistry Accounts, 2010, 125, 101-105.	1.4	0
36	Atmospheric reactivity of HCî€‚CCH2OH (2-propyn-1-ol) toward OH radicals: experimental determination and theoretical comparison with its alkyne analogue. RSC Advances, 2015, 5, 106668-106679.	3.6	0