Alexandra Simperler

List of Publications by Year
in descending order

26 papers	882 citations	471509 17 h-index	552781 26 g-index
26 all docs	26 docs citations	26 times ranked	1120 citing authors

#	Article	IF	Citations
1	Glass Transition Temperature of Glucose, Sucrose, and Trehalose:â€‰ An Experimental and in Silico Study. Journal of Physical Chemistry B, 2006, 110, 19678-19684.	2.6	136
2	Chemically feasible hypothetical crystalline networks. Nature Materials, 2004, 3, 234-238.	27.5	128
3	Taking the green fluorescence out of the protein: dynamics of the isolated GFP chromophore anion<sup />. Chemical Science, 2013, 4, 921-927.	7.4	75
4	Probing the Acid Strength of BrÃ¸nsted Acidic Zeolites with Acetonitrile:Â An Atomistic and Quantum Chemical Study. Journal of Physical Chemistry B, 2004, 108, 7152-7161.	2.6	58
5	Modeling the framework stability and catalytic activity of pure and transition metal-doped zeotypes. Journal of Solid State Chemistry, 2003, 176, 496-529.	2.9	50
6	Hypothetical Zeolitic Frameworks:â€‰ In Search of Potential Heterogeneous Catalysts. Journal of Physical Chemistry C, 2008, 112, 1040-1047.	3.1	46
7	Hypothetical binodal zeolitic frameworks. Acta Crystallographica Section B: Structural Science, 2005, 61, 263-279.	1.8	44
8	Intramolecular interactions in ortho-substituted phenols: survey of DFT-B3LYP calculated data. Journal of Molecular Structure, 1998, 448, 191-199.	3.6	39
9	Probing the Acid Strength of BrÃ¸nsted Acidic Zeolites with Acetonitrile:Â Quantum Chemical Calculation of1H,15N, and13C NMR Shift Parameters. Journal of Physical Chemistry B, 2004, 108, 7142-7151.	2.6	34
10	Correlation of melting points of inositols with hydrogen bonding patterns. CrystEngComm, 2006, 8, 589.	2.6	30
11	Adsorption of Methanol on Zeolites X and Y. An Atomistic and Quantum Chemical Study. Journal of Physical Chemistry B, 2006, 110, 6170-6178.	2.6	28
12	Theoretical Study of Toluene Adsorbed on Zeolites X and Y:â€‰ Calculation of 13C NMR Parameters. Journal of Physical Chemistry B, 2002, 106, 10944-10954.	2.6	26
13	Tetrahedral Distortion and Energetic Packing Penalty in â€œZeoliteâ€•Frameworks:Â Linked Phenomena?. Journal of Physical Chemistry B, 2005, 109, 14783-14785.	2.6	26
14	The glass transition temperatures of amorphous trehaloseâ€“water mixtures and the mobility of water: an experimental and in silico study. Carbohydrate Research, 2007, 342, 1470-1479.	2.3	25
15	Title is missing!. Catalysis Letters, 2003, 88, 163-167.	2.6	24
16	Hypothetical Uninodal Zeolite Structures:â€‰ Comparison of AlPO4 and SiO2 Compositions Using Computer Simulation. Journal of Physical Chemistry B, 2004, 108, 869-879.	2.6	21
17	Competition between photodetachment and autodetachment of the $m {2^1pi pi ^*}$21Ï€Ï€* state of the green fluorescent protein chromophore anion. Journal of Chemical Physics, 2014, 140, 205103.	3.0	21
18	A theoretical study of the reaction kinetics of amines released into the atmosphere from CO2 capture. International Journal of Greenhouse Gas Control, 2015, 41, 219-228.	4.6	15

#	Article	IF	Citations
19	Stability Series for the Complexation of Six Key Siderophore Functional Groups with Uranyl Using Density Functional Theory. Journal of Physical Chemistry A, 2020, 124, 2460-2472.	2.5	11
20	Evidence for heterodimers of 2,4,5-trichlorophenol on planar lipid layers. A FTIR-ATR investigation. Biochimica Et Biophysica Acta - Biomembranes, 2004, 1664, 88-99.	2.6	10
21	Computational Tools for Calculating log Î² Values of Geochemically Relevant Uranium Organometallic Complexes. Journal of Physical Chemistry A, 2018, 122, 8007-8019.	2.5	10
22	Defining the molecular properties of N-nitrosodimethylamine (NDMA) precursors using computational chemistry. Environmental Science: Water Research and Technology, 2017, 3, 502-512.	2.4	9
23	Lactonisationâ€"a degradation pathway for active pharmaceutical compounds: an in silico study in amorphous trehalose. Physical Chemistry Chemical Physics, 2007, 9, 3999-4006.	2.8	8
24	Atmospheric Chemistry Modelling of Amine Emissions from Post Combustion CO2 Capture Technology. Energy Procedia, 2014, 63, 822-829.	1.8	4
25	Competitive Hydrogen Bonds and Conformational Equilibria in Polysubstituted 3-Formyl-2-hydroxy-benzoyl Compounds. Monatshefte FÃ¼r Chemie, 2002, 133, 1337-1349.	1.8	3
26	Model study on the influence of plant design, photochemistry and meteorology on atmospheric concentrations of nitrosamines and nitramines in vicinity of an amine-based CO 2 capture facility. International Journal of Greenhouse Gas Control, 2017, 65, 203-217.	4.6	1