Krzysztof WoliÅ„ski

List of Publications by Year
in descending order

28 papers	6,930 citations	623188 14 h-index	552369 26 g-index
28 all docs	28 docs citations	28 times ranked	6514 citing authors

#	Article	IF	Citations
1	Efficient implementation of the gauge-independent atomic orbital method for NMR chemical shift calculations. Journal of the American Chemical Society, 1990, 112, 8251-8260.	6.6	6,130
2	Comparison of NMR Shieldings Calculated from Hartreeâ"Fock and Density Functional Wave Functions Using Gauge-Including Atomic Orbitals. The Journal of Physical Chemistry, 1996, 100, 6310-6316.	2.9	197
3	Quantum chemistry in parallel with PQS. Journal of Computational Chemistry, 2009, 30, 317-335.	1.5	104
4	Second-order MÃ¸llerâ€"Plesset calculations with dual basis sets. Journal of Chemical Physics, 2003, 118, 9497-9503.	1.2	98
5	Theoretical predictions of enforced structural changes in molecules. Molecular Physics, 2009, 107, 2403-2417.	0.8	75
6	Methods for parallel computation of SCF NMR chemical shifts by GIAO method: Efficient integral calculation, multi-Fock algorithm, and pseudodiagonalization. Journal of Computational Chemistry, 1997, 18, 816-825.	1.5	60
7	Quantum cluster equilibrium theory treatment of hydrogen-bonded liquids: water, methanol and ethanol. Molecular Physics, 2003, 101, 1413-1421.	0.8	41
8	Isomerization of stilbene using enforced geometry optimization. Journal of Computational Chemistry, 2011, 32, 43-53.	1.5	33
9	Geometry optimization in the presence of external forces: a theoretical model for enforced structural changes in molecules. Molecular Physics, 2010, 108, 1845-1856.	0.8	28
10	Magnetic shielding surface in molecules. Neutron as a probe in the hypothetical magnetic resonance spectroscopy. Journal of Chemical Physics, 1997, 106, 6061-6067.	1.2	26
11	Hartreeâ€"Fock and secondâ€order Mo/llerâ€"Plesset perturbation theory calculations of the31P nuclear magnetic resonance shielding tensor in PH3. Journal of Chemical Physics, 1993, 99, 7819-7824.	1.2	21
12	Recent developments in the PQS program. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 63-72.	6.2	17
13	Simulation of Force Spectroscopy Experiments on Galacturonic Acid Oligomers. PLoS ONE, 2014, 9, e107896.	1.1	17
14	The vibrational spectrum of 1,4-dioxane in aqueous solution â€" theory and experiment. New Journal of Chemistry, 2016, 40, 7663-7670.	1.4	16
15	Theoretical analysis of solvent effects on nitrogen NMR chemical shifts in oxazoles and oxadiazoles. Journal of Magnetic Resonance, 2009, 197, 153-160.	1.2	12
16	Kinetically stable high-energy isomers of C14H12 and C12H10N2 derived from cis-stilbene and cis-azobenzene. Journal of Molecular Modeling, 2011, 17, 1335-1342.	0.8	11
17	Parallel implementation of Hartreeâ€"Fock and density functional theory analytical second derivatives. Molecular Physics, 2004, 102, 2475-2484.	0.8	9
18	Exploring Potential Energy Surface with External Forces. Journal of Chemical Theory and Computation, 2018, 14, 6306-6316.	2.3	7

#	Article	IF	Citations
19	Theoretical studies of the pyranose ring under mechanical stress. Carbohydrate Research, 2018, 470, 64-72.	1.1	7
20	Molecular properties with dual basis set methods. Molecular Physics, 2008, 106, 769-786.	0.8	5
21	Isomerization and Decomposition of 2-Methylfuran with External Forces. Journal of Chemical Information and Modeling, 2019, 59, 3454-3463.	2.5	5
22	Solvent effects on the nitrogen NMR chemical shifts in 1-methylazoles â€“ a theoretical study. New Journal of Chemistry, 2015, 39, 9627-9640.	1.4	3
23	Driving proton transfer reactions in the 2-methylfuran ring with external forces. New Journal of Chemistry, 2020, 44, 8784-8795.	1.4	3
24	Simulation of the conformational flexibility of the mycodextran under external forces. Biopolymers, 2020, 111, e23357.	1.2	2
25	Protonation of Cytosine-Rich Telomeric DNA Fragments by Carboxylated Carbon Nanotubes: Insights from Computational Studies. Journal of Physical Chemistry B, 2021, 125, 5526-5536.	1.2	2
26	Approximate Force Constants from Uncoupled Self-Consistent Field Perturbation Theory Using Nonhybrid Density Functional Theory. Journal of Physical Chemistry A, 2017, 121, 348-356.	1.1	1
27	Compact representation of generalized molecular polarizabilities and efficient calculation of polarization energy in an arbitrary electric field. International Journal of Quantum Chemistry, 0, , e26792.	1.0	0
28	Search for transition states with external forces. Journal of Computational Chemistry, 2022, 43, 598-610.	1.5	0