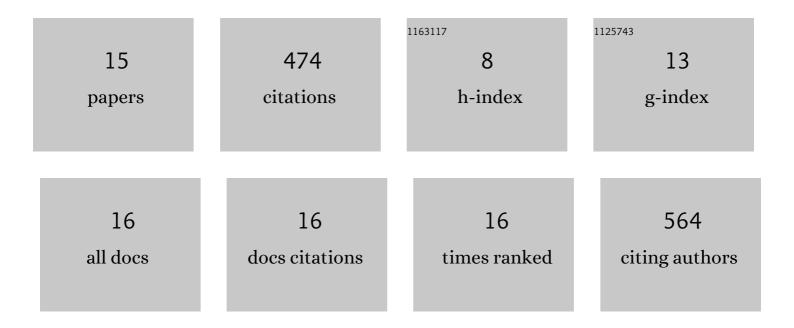
Bogdan Lesyng

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Generalized Born Model:Â Analysis, Refinement, and Applications to Proteins. Journal of Physical Chemistry B, 2004, 108, 18368-18376.	2.6	115
2	A comparative study of time dependent quantum mechanical wave packet evolution methods. Journal of Chemical Physics, 1992, 96, 2077-2084.	3.0	73
3	Ab initio study of proton transfer in [H3Nâ^'Hâ^'NH3]+ and [H3Nâ^'Hâ^'OH2]+. Chemical Physics Letters, 1990, 175, 282-288.	2.6	70
4	Class IV Charge Model for the Self-Consistent Charge Density-Functional Tight-Binding Method. Journal of Physical Chemistry A, 2004, 108, 2545-2549.	2.5	51
5	Molecular and electrostatic properties of the N-methylated nucleic acid bases by density functional theory. Chemical Physics, 1996, 204, 301-311.	1.9	42
6	Vibrations and hydrogen bonding in porphycene. Physical Chemistry Chemical Physics, 2012, 14, 5489.	2.8	41
7	Molecular modeling methods. Basic techniques and challenging problems. , 1993, 60, 149-167.		29
8	Carâ^'Parrinello Molecular Dynamics Study of the Intramolecular Vibrational Mode-Sensitive Double Proton-Transfer Mechanisms in Porphycene. Journal of Physical Chemistry A, 2010, 114, 2313-2318.	2.5	28
9	Energy minimization and molecular dynamics studies of Asn-102 elastase. Journal of Computer-Aided Molecular Design, 1987, 1, 211-217.	2.9	8
10	Hydration free energy of a Model Lennard-Jones solute particle: Microscopic Monte Carlo simulation studies, and interpretation based on mesoscopic models. Journal of Chemical Physics, 2008, 128, 064503.	3.0	5
11	Thermal Fluctuations and Infrared Spectra of the Formamide–Formamidine Complex. Journal of Physical Chemistry A, 2012, 116, 10412-10419.	2.5	4
12	Exploring Covalent Docking Mechanisms of Boron-Based Inhibitors to Class A, C and D β-Lactamases Using Time-dependent Hybrid QM/MM Simulations. Frontiers in Molecular Biosciences, 2021, 8, 633181.	3.5	4
13	Selected Microscopic and Mezoscopic Modelling Tools and Models – an Overview. Challenges and Advances in Computational Chemistry and Physics, 2007, , 203-223.	0.6	2
14	Parallel version of a quantum classical molecular dynamics code for complex molecular and biomolecular systems. Lecture Notes in Computer Science, 1997, , 409-416.	1.3	2
15	A novel formulation of an approximate valence bond model (AVB2) and its application to the tautomeric forms of porphyrin and porphycene. Journal of Molecular Modeling, 2019, 25, 155.	1.8	0