Bogdan Lesyng

List of Publications by Year
in descending order

15	474	1163117 8	1125743 13
papers	citations	h-index	g-index

16	16	16	564
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Exploring Covalent Docking Mechanisms of Boron-Based Inhibitors to Class A, C and D Î²-Lactamases Using Time-dependent Hybrid QM/MM Simulations. Frontiers in Molecular Biosciences, 2021, 8, 633181.	3.5	4
2	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
3	Vibrations and hydrogen bonding in porphycene. Physical Chemistry Chemical Physics, 2012, 14, 5489.	2.8	41
4	Thermal Fluctuations and Infrared Spectra of the Formamideâ€“Formamidine Complex. Journal of Physical Chemistry A, 2012, 116, 10412-10419.	2.5	4
5	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
6	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
7	Selected Microscopic and Mezoscopic Modelling Tools and Models â€“ an Overview. Challenges and Advances in Computational Chemistry and Physics, 2007, , 203-223.	0.6	2
8	Generalized Born Model:Â Analysis, Refinement, and Applications to Proteins. Journal of Physical Chemistry B, 2004, 108, 18368-18376.	2.6	115
9	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
10	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
11	Molecular and electrostatic properties of the N-methylated nucleic acid bases by density functional theory. Chemical Physics, 1996, 204, 301-311.	1.9	42
12	Molecular modeling methods. Basic techniques and challenging problems. , 1993, 60, 149-167.		29
13	A comparative study of time dependent quantum mechanical wave packet evolution methods. Journal of Chemical Physics, 1992, 96, 2077-2084.	3.0	73
14	Ab initio study of proton transfer in [H3Nâ€'Hâ€'NH3]+ and [H3Nâ€'Hâ€'OH2]+. Chemical Physics Letters, 1990, 175, 282-288.	2.6	70
15	Energy minimization and molecular dynamics studies of Asn-102 elastase. Journal of Computer-Aided Molecular Design, 1987, 1, 211-217.	2.9	8