Volodymyr Babin

List of Publications by Year
in descending order

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29 papers	2,218 citations	430843 18 h-index	454934 30 g-index
31 all docs	31 docs citations	31 times ranked	1848 citing authors

#	Article	IF	Citations
1	Development of a â€œFirst Principlesâ€•Water Potential with Flexible Monomers: Dimer Potential Energy Surface, VRT Spectrum, and Second Virial Coefficient. Journal of Chemical Theory and Computation, 2013, 9, 5395-5403.	5.3	398
2	Development of a â€œFirst Principlesâ€•Water Potential with Flexible Monomers. II: Trimer Potential Energy Surface, Third Virial Coefficient, and Small Clusters. Journal of Chemical Theory and Computation, 2014, 10, 1599-1607.	5.3	313
3	Development of a â€œFirst-Principlesâ€•Water Potential with Flexible Monomers. III. Liquid Phase Properties. Journal of Chemical Theory and Computation, 2014, 10, 2906-2910.	5.3	292
4	Adaptively biased molecular dynamics for free energy calculations. Journal of Chemical Physics, 2008, 128, 134101.	3.0	168
5	Toward a Universal Water Model: First Principles Simulations from the Dimer to the Liquid Phase. Journal of Physical Chemistry Letters, 2012, 3, 3765-3769.	4.6	137
6	The Water Hexamer: Cage, Prism, or Both. Full Dimensional Quantum Simulations Say Both. Journal of the American Chemical Society, 2012, 134, 11116-11119.	13.7	132
7	A Critical Assessment of Two-Body and Three-Body Interactions in Water. Journal of Chemical Theory and Computation, 2013, 9, 1103-1114.	5.3	126
8	Conformations and free energy landscapes of polyproline peptides. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 20746-20751.	7.1	92
9	The free energy landscape of small peptides as obtained from metadynamics with umbrella sampling corrections. Journal of Chemical Physics, 2006, 125, 204909.	3.0	74
10	Molecular Dynamics Simulations of DNA with Polarizable Force Fields:Â Convergence of an Ideal B-DNA Structure to the Crystallographic Structure. Journal of Physical Chemistry B, 2006, 110, 11571-11581.	2.6	65
11	Deprotonation of Solvated Formic Acid:Â Carâ˜Parrinello and Metadynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 2325-2331.	2.6	51
12	Conformational free energies of methyl-Î±-L-iduronic and methyl-Î²-D-glucuronic acids in water. Journal of Chemical Physics, 2010, 132, 104108.	3.0	49
13	Reaction path ensemble of the Bâ€“Z-DNA transition: a comprehensive atomistic study. Nucleic Acids Research, 2013, 41, 33-43.	14.5	48
14	The curious case of the water hexamer: Cage vs. Prism. Chemical Physics Letters, 2013, 580, 1-8.	2.6	41
15	Adaptively biased molecular dynamics: An umbrella sampling method with a timeâ€dependent potential. International Journal of Quantum Chemistry, 2009, 109, 3666-3678.	2.0	35
16	A classical molecular dynamics investigation of the free energy and structure of short polyproline conformers. Journal of Chemical Physics, 2010, 133, 125104.	3.0	32
17	A Statistical Analysis of the PPII Propensity of Amino Acid Guests in Proline-Rich Peptides. Biophysical Journal, 2011, 100, 1083-1093.	0.5	24
18	The Î±â€sheet: A missingâ€inâ€action secondary structure?. Proteins: Structure, Function and Bioinformatics, 2011, 79, 937-946.	2.6	19

#	Article	IF	Citations
19	Are Long-Range Structural Correlations Behind the Aggregration Phenomena of Polyglutamine Diseases?. PLoS Computational Biology, 2012, 8, e1002501.	3.2	18
20	PPII Propensity of Multiple-Guest Amino Acids in a Proline-Rich Environment. Journal of Physical Chemistry B, 2011, 115, 8645-8656.	2.6	17
21	Free energy and structure of polyproline peptides: An ab initio and classical molecular dynamics investigation. International Journal of Quantum Chemistry, 2010, 110, 2865-2879.	2.0	16
22	Molecular dynamics simulations of polarizable DNA in crystal environment. International Journal of Quantum Chemistry, 2006, 106, 3260-3269.	2.0	12
23	The Adaptively Biased Molecular Dynamics method revisited: New capabilities and an application. Journal of Physics: Conference Series, 2015, 640, 012020.	0.4	12
24	Minimization of the Renyi entropy production in the stationary states of the Brownian process with matched death and birth rates. Physical Review E, 2004, 69, 016110.	2.1	10
25	Binding Polymorphism in the DNA Bound State of the Pdx1 Homeodomain. PLoS Computational Biology, 2013, 9, e1003160.	3.2	9
26	Pattern formation in nonextensive thermodynamics: Selection criterion based on the Renyi entropy production. Journal of Chemical Physics, 2005, 122, 174105.	3.0	8
27	Electrostatics Interactions in Classical Simulations. Methods in Molecular Biology, 2013, 924, 243-270.	0.9	8
28	Recipes for Free Energy Calculations in Biomolecular Systems. Methods in Molecular Biology, 2013, 924, 313-337.	0.9	6
29	Low-temperature isomers of the water hexamer as predicted by q-TIP4P/F and TTM3-F potentials. , 2013, , .		0