Volodymyr Babin

List of Publications by Citations

28 papers	1,808 citations	17 h-index	31 g-index
31 ext. papers	2,030 ext. citations	4.8 avg, IF	5.01 L-index

#	Paper	IF	Citations
28	Development of a "First Principles" Water Potential with Flexible Monomers: Dimer Potential Energy Surface, VRT Spectrum, and Second Virial Coefficient. *Journal of Chemical Theory and Computation*, **2013**, 9, 5395-403	6.4	296
27	Development of a "First Principles" Water Potential with Flexible Monomers. II: Trimer Potential Energy Surface, Third Virial Coefficient, and Small Clusters. *Journal of Chemical Theory and Computation*, **2014**, 10, 1599-607	6.4	230
26	Development of a "First-Principles" Water Potential with Flexible Monomers. III. Liquid Phase Properties. *Journal of Chemical Theory and Computation*, **2014**, 10, 2906-10	6.4	227
25	Adaptively biased molecular dynamics for free energy calculations. *Journal of Chemical Physics*, **2008**, 128, 134101	3.9	138
24	Toward a Universal Water Model: First Principles Simulations from the Dimer to the Liquid Phase. *Journal of Physical Chemistry Letters*, **2012**, 3, 3765-9	6.4	114
23	The water hexamer: cage, prism, or both. Full dimensional quantum simulations say both. *Journal of the American Chemical Society*, **2012**, 134, 11116-9	16.4	114
22	A Critical Assessment of Two-Body and Three-Body Interactions in Water. *Journal of Chemical Theory and Computation*, **2013**, 9, 1103-14	6.4	111
21	Conformations and free energy landscapes of polyproline peptides. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 20746-51	11.5	80
20	The free energy landscape of small peptides as obtained from metadynamics with umbrella sampling corrections. *Journal of Chemical Physics*, **2006**, 125, 204909	3.9	72
19	Molecular dynamics simulations of DNA with polarizable force fields: convergence of an ideal B-DNA structure to the crystallographic structure. *Journal of Physical Chemistry B*, **2006**, 110, 11571-81	3.4	62
18	Deprotonation of solvated formic acid: Car-Parrinello and metadynamics simulations. *Journal of Physical Chemistry B*, **2006**, 110, 2325-31	3.4	49
17	Conformational free energies of methyl-alpha-L-iduronic and methyl-beta-D-glucuronic acids in water. *Journal of Chemical Physics*, **2010**, 132, 104108	3.9	44
16	Reaction path ensemble of the B-Z-DNA transition: a comprehensive atomistic study. *Nucleic Acids Research*, **2013**, 41, 33-43	20.1	39
15	The curious case of the water hexamer: Cage vs. Prism. *Chemical Physics Letters*, **2013**, 580, 1-8	2.5	36
14	A classical molecular dynamics investigation of the free energy and structure of short polyproline conformers. *Journal of Chemical Physics*, **2010**, 133, 125104	3.9	29
13	Adaptively biased molecular dynamics: An umbrella sampling method with a time-dependent potential. *International Journal of Quantum Chemistry*, **2009**, 109, 3666-3678	2.1	27
12	A statistical analysis of the PPII propensity of amino acid guests in proline-rich peptides. *Biophysical Journal*, **2011**, 100, 1083-93	2.9	23

11	The β-sheet: a missing-in-action secondary structure?. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 937-46	4.2	17
10	PPII propensity of multiple-guest amino acids in a proline-rich environment. *Journal of Physical Chemistry B*, **2011**, 115, 8645-56	3.4	15
9	Free energy and structure of polyproline peptides: An ab initio and classical molecular dynamics investigation. *International Journal of Quantum Chemistry*, **2010**, 110, 2865-2879	2.1	15
8	Are long-range structural correlations behind the aggregration phenomena of polyglutamine diseases?. *PLoS Computational Biology*, **2012**, 8, e1002501	5	14
7	Molecular dynamics simulations of polarizable DNA in crystal environment. *International Journal of Quantum Chemistry*, **2006**, 106, 3260-3269	2.1	12
6	The Adaptively Biased Molecular Dynamics method revisited: New capabilities and an application. *Journal of Physics: Conference Series*, **2015**, 640, 012020	0.3	8
5	Binding polymorphism in the DNA bound state of the Pdx1 homeodomain. *PLoS Computational Biology*, **2013**, 9, e1003160	5	8
4	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	2.4	8
3	Electrostatics interactions in classical simulations. *Methods in Molecular Biology*, **2013**, 924, 243-70	1.4	6
2	Recipes for free energy calculations in biomolecular systems. *Methods in Molecular Biology*, **2013**, 924, 313-37	1.4	5
1	Pattern formation in nonextensive thermodynamics: selection criterion based on the Renyi entropy production. *Journal of Chemical Physics*, **2005**, 122, 174105	3.9	4