Pavel BanÃ¡Å¡

List of Publications by Year
in descending order

69 papers	5,748 citations	94433 37 h-index	82547 72 g-index
78 all docs	78 docs citations	78 times ranked	5336 citing authors

#	Article	IF	Citations
1	Early steps of oxidative damage in DNA quadruplexes are position-dependent: Quantum mechanical and molecular dynamics analysis of human telomeric sequence containing ionized guanine. International Journal of Biological Macromolecules, 2022, 194, 882-894.	7.5	2
2	Toward Convergence in Folding Simulations of RNA Tetraloops: Comparison of Enhanced Sampling Techniques and Effects of Force Field Modifications. Journal of Chemical Theory and Computation, 2022, 18, 2642-2656.	5.3	34
3	Automatic Learning of Hydrogen-Bond Fixes in the AMBER RNA Force Field. Journal of Chemical Theory and Computation, 2022, 18, 4490-4502.	5.3	21
4	W-RESP: Well-Restrained Electrostatic Potential-Derived Charges. Revisiting the Charge Derivation Model. Journal of Chemical Theory and Computation, 2021, 17, 3495-3509.	5.3	18
5	Molecular insights from theoretical calculations explain the differences in affinity and diffusion of airborne contaminants on surfaces of hBN and graphene. Applied Surface Science, 2021, 565, 150382.	6.1	2
6	UUCG RNA Tetraloop as a Formidable Force-Field Challenge for MD Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7601-7617.	5.3	29
7	Fine-Tuning of the AMBER RNA Force Field with a New Term Adjusting Interactions of Terminal Nucleotides. Journal of Chemical Theory and Computation, 2020, 16, 3936-3946.	5.3	39
8	Parallel G-triplexes and G-hairpins as potential transitory ensembles in the folding of parallel-stranded DNA G-Quadruplexes. Nucleic Acids Research, 2019, 47, 7276-7293.	14.5	42
9	Variability of Câ€“F Bonds Governs the Formation of Specific Structural Motifs in Fluorinated Graphenes. Journal of Physical Chemistry C, 2019, 123, 27896-27903.	3.1	22
10	Local-to-global signal transduction at the core of a Mn2+ sensing riboswitch. Nature Communications, 2019, 10, 4304.	12.8	24
11	Fitting Corrections to an RNA Force Field Using Experimental Data. Journal of Chemical Theory and Computation, 2019, 15, 3425-3431.	5.3	54
12	Improving the Performance of the Amber RNA Force Field by Tuning the Hydrogen-Bonding Interactions. Journal of Chemical Theory and Computation, 2019, 15, 3288-3305.	5.3	97
13	Ion Interactions across Graphene in Electrolyte Aqueous Solutions. Journal of Physical Chemistry C, 2019, 123, 9799-9806.	3.1	25
14	Investigations of Stacked DNA Base-Pair Steps: Highly Accurate Stacking Interaction Energies, Energy Decomposition, and Many-Body Stacking Effects. Journal of Chemical Theory and Computation, 2019, 15, 95-115.	5.3	55
15	RNA Structural Dynamics As Captured by Molecular Simulations: A Comprehensive Overview. Chemical Reviews, 2018, 118, 4177-4338.	47.7	408
16	Structural dynamics of propeller loop: towards folding of RNA G-quadruplex. Nucleic Acids Research, 2018, 46, 8754-8771.	14.5	29
17	Exploring the Dynamics of Propeller Loops in Human Telomeric DNA Quadruplexes Using Atomistic Simulations. Journal of Chemical Theory and Computation, 2017, 13, 2458-2480.	5.3	39
18	Noncanonical Î±/Î³ Backbone Conformations in RNA and the Accuracy of Their Description by the AMBER Force Field. Journal of Physical Chemistry B, 2017, 121, 2420-2433.	2.6	27

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19	Folding of guanine quadruplex moleculesâ€“funnel-like mechanism or kinetic partitioning? An overview from MD simulation studies. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 1246-1263.	2.4	89
20	Mapping the Chemical Space of the RNA Cleavage and Its Implications for Ribozyme Catalysis. Journal of Physical Chemistry B, 2017, 121, 10828-10840.	2.6	4
21	How to understand atomistic molecular dynamics simulations of <scp>RNA</scp> and proteinâ€“<scp>RNA</scp> complexes?. Wiley Interdisciplinary Reviews RNA, 2017, 8, e1405.	6.4	54
22	Free Energy Landscape of GAGA and UUCG RNA Tetraloops. Journal of Physical Chemistry Letters, 2016, 7, 4032-4038.	4.6	70
23	Exponential repulsion improves structural predictability of molecular docking. Journal of Computational Chemistry, 2016, 37, 2485-2494.	3.3	8
24	Computer Folding of RNA Tetraloops: Identification of Key Force Field Deficiencies. Journal of Chemical Theory and Computation, 2016, 12, 4534-4548.	5.3	125
25	Microsecond-Scale MD Simulations of HIV-1 DIS Kissing-Loop Complexes Predict Bulged-In Conformation of the Bulged Bases and Reveal Interesting Differences between Available Variants of the AMBER RNA Force Fields. Journal of Physical Chemistry B, 2015, 119, 15176-15190.	2.6	20
26	The role of an active site Mg²⁺ in HDV ribozyme self-cleavage: insights from QM/MM calculations. Physical Chemistry Chemical Physics, 2015, 17, 670-679.	2.8	28
27	Insights into Stability and Folding of GNRA and UNCG Tetraloops Revealed by Microsecond Molecular Dynamics and Well-Tempered Metadynamics. Journal of Chemical Theory and Computation, 2015, 11, 3866-3877.	5.3	60
28	Reactivity of Fluorographene: A Facile Way toward Graphene Derivatives. Journal of Physical Chemistry Letters, 2015, 6, 1430-1434.	4.6	90
29	Reactive Conformation of the Active Site in the Hairpin Ribozyme Achieved by Molecular Dynamics Simulations with Îµ/Î¶ Force Field Reparametrizations. Journal of Physical Chemistry B, 2015, 119, 4220-4229.	2.6	45
30	Chemical feasibility of the general acid/base mechanism of glmS ribozyme selfâ€cleavage. Biopolymers, 2015, 103, 550-562.	2.4	9
31	Hairpins participating in folding of human telomeric sequence quadruplexes studied by standard and T-REMD simulations. Nucleic Acids Research, 2015, 43, gkv994.	14.5	47
32	Interplay between Ethanol Adsorption to High-Energy Sites and Clustering on Graphene and Graphite Alters the Measured Isosteric Adsorption Enthalpies. Journal of Physical Chemistry C, 2015, 119, 20535-20543.	3.1	31
33	Wobble pairs of the HDV ribozyme play specific roles in stabilization of active site dynamics. Physical Chemistry Chemical Physics, 2015, 17, 5887-5900.	2.8	6
34	Molecular dynamic simulations of protein/RNA complexes: CRISPR/Csy4 endoribonuclease. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 1072-1090.	2.4	20
35	Anatomy of enzyme channels. BMC Bioinformatics, 2014, 15, 379.	2.6	89
36	The nature of high surface energy sites in graphene and graphite. Carbon, 2014, 73, 448-453.	10.3	38

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37	Molecular Dynamics Simulations of Nucleic Acids. From Tetranucleotides to the Ribosome. Journal of Physical Chemistry Letters, 2014, 5, 1771-1782.	4.6	139
38	Comparison of ab Initio, DFT, and Semiempirical QM/MM Approaches for Description of Catalytic Mechanism of Hairpin Ribozyme. Journal of Chemical Theory and Computation, 2014, 10, 1608-1622.	5.3	56
39	Energies and 2â€²-Hydroxyl Group Orientations of RNA Backbone Conformations. Benchmark CCSD(T)/CBS Database, Electronic Analysis, and Assessment of DFT Methods and MD Simulations. Journal of Chemical Theory and Computation, 2014, 10, 463-480.	5.3	24
40	Are Waters around RNA More than Just a Solvent? â€“ An Insight from Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2014, 10, 401-411.	5.3	33
41	Disparate HDV ribozyme crystal structures represent intermediates on a rugged free-energy landscape. Rna, 2014, 20, 1112-1128.	3.5	15
42	Nature and magnitude of aromatic base stacking in DNA and RNA: Quantum chemistry, molecular mechanics, and experiment. Biopolymers, 2013, 99, 978-988.	2.4	106
43	MOLE 2.0: advanced approach for analysis of biomacromolecular channels. Journal of Cheminformatics, 2013, 5, 39.	6.1	262
44	Effect of Guanine to Inosine Substitution on Stability of Canonical DNA and RNA Duplexes: Molecular Dynamics Thermodynamics Integration Study. Journal of Physical Chemistry B, 2013, 117, 1872-1879.	2.6	42
45	Computer Folding of RNA Tetraloops? Are We There Yet?. Journal of Chemical Theory and Computation, 2013, 9, 2115-2125.	5.3	84
46	Benchmark quantum-chemical calculations on a complete set of rotameric families of the DNA sugarâ€“phosphate backbone and their comparison with modern density functional theory. Physical Chemistry Chemical Physics, 2013, 15, 7295.	2.8	33
47	How to understand quantum chemical computations on DNA and RNA systems? A practical guide for non-specialists. Methods, 2013, 64, 3-11.	3.8	45
48	MOLEonline 2.0: interactive web-based analysis of biomacromolecular channels. Nucleic Acids Research, 2012, 40, W222-W227.	14.5	123
49	Reference Simulations of Noncanonical Nucleic Acids with Different Ï‡ Variants of the AMBER Force Field: Quadruplex DNA, Quadruplex RNA, and Z-DNA. Journal of Chemical Theory and Computation, 2012, 8, 2506-2520.	5.3	231
50	The DNA and RNA sugarâ€“phosphate backbone emerges as the key player. An overview of quantum-chemical, structural biology and simulation studies. Physical Chemistry Chemical Physics, 2012, 14, 15257.	2.8	76
51	Can We Accurately Describe the Structure of Adenine Tracts in B-DNA? Reference Quantum-Chemical Computations Reveal Overstabilization of Stacking by Molecular Mechanics. Journal of Chemical Theory and Computation, 2012, 8, 2448-2460.	5.3	67
52	Molecular Mechanism of preQ₁ Riboswitch Action: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2012, 116, 12721-12734.	2.6	43
53	Simulations of A-RNA Duplexes. The Effect of Sequence, Solute Force Field, Water Model, and Salt Concentration. Journal of Physical Chemistry B, 2012, 116, 9899-9916.	2.6	64
54	Understanding RNA Flexibility Using Explicit Solvent Simulations: The Ribosomal and Group I Intron Reverse Kink-Turn Motifs. Journal of Chemical Theory and Computation, 2011, 7, 2963-2980.	5.3	49

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55	Refinement of the Cornell et al. Nucleic Acids Force Field Based on Reference Quantum Chemical Calculations of Glycosidic Torsion Profiles. Journal of Chemical Theory and Computation, 2011, 7, 2886-2902.	5.3	873
56	QM/MM Studies of Hairpin Ribozyme Self-Cleavage Suggest the Feasibility of Multiple Competing Reaction Mechanisms. Journal of Physical Chemistry B, 2011, 115, 13911-13924.	2.6	33
57	Theoretical Studies on the Intermolecular Interactions of Potentially Primordial Baseâ€Pair Analogues. Chemistry - A European Journal, 2010, 16, 3057-3065.	3.3	13
58	Extensive Molecular Dynamics Simulations Showing That Canonical G8 and Protonated A38H⁺ Forms Are Most Consistent with Crystal Structures of Hairpin Ribozyme. Journal of Physical Chemistry B, 2010, 114, 6642-6652.	2.6	81
59	Explicit Water Models Affect the Specific Solvation and Dynamics of Unfolded Peptides While the Conformational Behavior and Flexibility of Folded Peptides Remain Intact. Journal of Chemical Theory and Computation, 2010, 6, 3569-3579.	5.3	108
60	Protonation States of the Key Active Site Residues and Structural Dynamics of the glmS Riboswitch As Revealed by Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 8701-8712.	2.6	54
61	Performance of Molecular Mechanics Force Fields for RNA Simulations: Stability of UUCG and GNRA Hairpins. Journal of Chemical Theory and Computation, 2010, 6, 3836-3849.	5.3	339
62	Redesigning dehalogenase access tunnels as a strategy for degrading an anthropogenic substrate. Nature Chemical Biology, 2009, 5, 727-733.	8.0	238
63	Theoretical studies of RNA catalysis: Hybrid QM/MM methods and their comparison with MD and QM. Methods, 2009, 49, 202-216.	3.8	82
64	Two C-terminal ankyrin repeats form the minimal stable unit of the ankyrin repeat protein p18INK4c. Journal of Molecular Modeling, 2008, 14, 747-759.	1.8	6
65	Second step of hydrolytic dehalogenation in haloalkane dehalogenase investigated by QM/MM methods. Proteins: Structure, Function and Bioinformatics, 2008, 70, 707-717.	2.6	24
66	General Base Catalysis for Cleavage by the Active-Site Cytosine of the Hepatitis Delta Virus Ribozyme: QM/MM Calculations Establish Chemical Feasibility. Journal of Physical Chemistry B, 2008, 112, 11177-11187.	2.6	46
67	Identification of tunnels in proteins, nucleic acids, inorganic materials and molecular ensembles. Biotechnology Journal, 2007, 2, 62-67.	3.5	53
68	Mechanism of enhanced conversion of 1,2,3-trichloropropane by mutant haloalkane dehalogenase revealed by molecular modeling. Journal of Computer-Aided Molecular Design, 2006, 20, 375-383.	2.9	25
69	CAVER: a new tool to explore routes from protein clefts, pockets and cavities. BMC Bioinformatics, 2006, 7, 316.	2.6	453