Petr JureÄka

List of Publications by Year in descending order

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47 papers	8,002 citations	136950 32 h-index	206112 48 g-index
50 all docs	50 docs citations	50 times ranked	7077 citing authors

#	Article	IF	Citations
1	The <scp>Adâ€MD</scp> method to calculate <scp>NMR</scp> shift including effects due to conformational dynamics: The <scp>³¹P NMR</scp> shift in <scp>DNA</scp>. Journal of Computational Chemistry, 2022, 43, 132-143.	3.3	5
2	Conformational energies and equilibria of cyclic dinucleotidesin vacuoand in solution: computational chemistryvs.NMR experiments. Physical Chemistry Chemical Physics, 2021, 23, 7280-7294.	2.8	5
3	Z-DNA as a Touchstone for Additive Empirical Force Fields and a Refinement of the Alpha/Gamma DNA Torsions for AMBER. Journal of Chemical Theory and Computation, 2021, 17, 6292-6301.	5.3	30
4	Toward Accurate Hydrogen Bonds by Scalable Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2019, 15, 3552-3557.	5.3	12
5	RNA Structural Dynamics As Captured by Molecular Simulations: A Comprehensive Overview. Chemical Reviews, 2018, 118, 4177-4338.	47.7	408
6	A- to B-DNA Transition in AMBER Force Fields and Its Coupling to Sugar Pucker. Journal of Chemical Theory and Computation, 2018, 14, 319-328.	5.3	22
7	Influence of BII Backbone Substates on DNA Twist: A Unified View and Comparison of Simulation and Experiment for All 136 Distinct Tetranucleotide Sequences. Journal of Chemical Information and Modeling, 2017, 57, 275-287.	5.4	31
8	Adsorption of Organic Molecules to van der Waals Materials: Comparison of Fluorographene and Fluorographite with Graphene and Graphite. Journal of Chemical Theory and Computation, 2017, 13, 1328-1340.	5.3	47
9	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
10	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
11	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
12	Noncovalent Interactions by Quantum Monte Carlo. Chemical Reviews, 2016, 116, 5188-5215.	47.7	114
13	Assessing the Current State of Amber Force Field Modifications for DNA. Journal of Chemical Theory and Computation, 2016, 12, 4114-4127.	5.3	351
14	On the Use of Molecular Dynamics Simulations for Probing Allostery through DNA. Biophysical Journal, 2016, 110, 874-876.	0.5	14
15	Modelling of graphene functionalization. Physical Chemistry Chemical Physics, 2016, 18, 6351-6372.	2.8	190
16	Transferability and additivity of dihedral parameters in polarizable and nonpolarizable empirical force fields. Journal of Computational Chemistry, 2015, 36, 1874-1884.	3.3	15
17	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
18	Extensions and applications of the A24 data set of accurate interaction energies. Physical Chemistry Chemical Physics, 2015, 17, 19268-19277.	2.8	50

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19	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
20	Refinement of the Sugarâ€“Phosphate Backbone Torsion Beta for AMBER Force Fields Improves the Description of Z- and B-DNA. Journal of Chemical Theory and Computation, 2015, 11, 5723-5736.	5.3	392
21	Mechanical properties of symmetric and asymmetric DNA A-tracts: implications for looping and nucleosome positioning. Nucleic Acids Research, 2014, 42, 7383-7394.	14.5	59
22	Molecular Dynamics Simulations of Nucleic Acids. From Tetranucleotides to the Ribosome. Journal of Physical Chemistry Letters, 2014, 5, 1771-1782.	4.6	139
23	Mechanical Model of DNA Allostery. Journal of Physical Chemistry Letters, 2014, 5, 3831-3835.	4.6	24
24	Base Pair Fraying in Molecular Dynamics Simulations of DNA and RNA. Journal of Chemical Theory and Computation, 2014, 10, 3177-3189.	5.3	135
25	Quantum Monte Carlo for noncovalent interactions: an efficient protocol attaining benchmark accuracy. Physical Chemistry Chemical Physics, 2014, 16, 20915-20923.	2.8	46
26	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
27	Toward Improved Description of DNA Backbone: Revisiting Epsilon and Zeta Torsion Force Field Parameters. Journal of Chemical Theory and Computation, 2013, 9, 2339-2354.	5.3	255
28	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
29	Quantum Monte Carlo Methods Describe Noncovalent Interactions with Subchemical Accuracy. Journal of Chemical Theory and Computation, 2013, 9, 4287-4292.	5.3	88
30	Adsorption of Small Organic Molecules on Graphene. Journal of the American Chemical Society, 2013, 135, 6372-6377.	13.7	407
31	Lipid Enhanced Exfoliation for Production of Graphene Nanosheets. Journal of Physical Chemistry C, 2013, 117, 11800-11803.	3.1	38
32	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
33	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
34	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
35	A Novel Approach for Deriving Force Field Torsion Angle Parameters Accounting for Conformation-Dependent Solvation Effects. Journal of Chemical Theory and Computation, 2012, 8, 3232-3242.	5.3	27
36	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

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37	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
38	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
39	Large-scale compensation of errors in pairwise-additive empirical force fields: comparison of AMBER intermolecular terms with rigorous DFT-SAPT calculations. Physical Chemistry Chemical Physics, 2010, 12, 10476.	2.8	79
40	Reference Quantum Chemical Calculations on RNA Base Pairs Directly Involving the 2â€²-OH Group of Ribose. Journal of Chemical Theory and Computation, 2009, 5, 1166-1179.	5.3	27
41	Theoretical studies of RNA catalysis: Hybrid QM/MM methods and their comparison with MD and QM. Methods, 2009, 49, 202-216.	3.8	82
42	Balance of Attraction and Repulsion in Nucleic-Acid Base Stacking: CCSD(T)/Complete-Basis-Set-Limit Calculations on Uracil Dimer and a Comparison with the Force-Field Description. Journal of Chemical Theory and Computation, 2009, 5, 1524-1544.	5.3	51
43	Understanding of Assembly Phenomena by Aromaticâ"Aromatic Interactions:Â Benzene Dimer and the Substituted Systems. Journal of Physical Chemistry A, 2007, 111, 3446-3457.	2.5	617
44	Benchmark database of accurate (MP2 and CCSD(T) complete basis set limit) interaction energies of small model complexes, DNA base pairs, and amino acid pairs. Physical Chemistry Chemical Physics, 2006, 8, 1985-1993.	2.8	1,635
45	True Stabilization Energies for the Optimal Planar Hydrogen-Bonded and Stacked Structures of GuanineÂ·Â·Â·Cytosine, AdenineÂ·Â·Â·Thymine, and Their 9- and 1-Methyl Derivatives:â€‰ Complete Basis Set Calculations at the MP2 and CCSD(T) Levels and Comparison with Experiment. Journal of the American Chemical Society, 2003, 125, 15608-15613.	13.7	353
46	On the convergence of the (Î"ECCSD(T)â^'Î"EMP2) term for complexes with multiple H-bonds. Chemical Physics Letters, 2002, 365, 89-94.	2.6	235
47	RI-MP2 calculations with extended basis setsÃ¢â‚¬â„¢ promising tool for study of H-bonded and stacked DNA base pairs. Physical Chemistry Chemical Physics, 2001, 3, 4578-4582.	2.8	106