Petr JureÄka

List of Publications by Year in descending order

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47	8,002	136885	206029
papers	citations	32	48
		h-index	g-index

50	50	50	7077
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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.	1.3	1,635
2	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.	2.3	873
3	Understanding of Assembly Phenomena by Aromaticâ^'Aromatic Interactions:Â Benzene Dimer and the Substituted Systems. Journal of Physical Chemistry A, 2007, 111, 3446-3457.	1.1	617
4	RNA Structural Dynamics As Captured by Molecular Simulations: A Comprehensive Overview. Chemical Reviews, 2018, 118, 4177-4338.	23.0	408
5	Adsorption of Small Organic Molecules on Graphene. Journal of the American Chemical Society, 2013, 135, 6372-6377.	6.6	407
6	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.	2.3	392
7	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.	6.6	353
8	Assessing the Current State of Amber Force Field Modifications for DNA. Journal of Chemical Theory and Computation, 2016, 12, 4114-4127.	2.3	351
9	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.	2.3	339
10	Toward Improved Description of DNA Backbone: Revisiting Epsilon and Zeta Torsion Force Field Parameters. Journal of Chemical Theory and Computation, 2013, 9, 2339-2354.	2.3	255
11	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.	1.2	235
12	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.	2.3	231
13	Modelling of graphene functionalization. Physical Chemistry Chemical Physics, 2016, 18, 6351-6372.	1.3	190
14	Molecular Dynamics Simulations of Nucleic Acids. From Tetranucleotides to the Ribosome. Journal of Physical Chemistry Letters, 2014, 5, 1771-1782.	2.1	139
15	Base Pair Fraying in Molecular Dynamics Simulations of DNA and RNA. Journal of Chemical Theory and Computation, 2014, 10, 3177-3189.	2.3	135
16	Noncovalent Interactions by Quantum Monte Carlo. Chemical Reviews, 2016, 116, 5188-5215.	23.0	114
17	RI-MP2 calculations with extended basis setsÃ¢â‚¬â€œ promising tool for study of H-bonded and stacked DNA base pairs. Physical Chemistry Chemical Physics, 2001, 3, 4578-4582.	1.3	106
18	Nature and magnitude of aromatic base stacking in DNA and RNA: Quantum chemistry, molecular mechanics, and experiment. Biopolymers, 2013, 99, 978-988.	1.2	106

#	Article	IF	Citations
19	Quantum Monte Carlo Methods Describe Noncovalent Interactions with Subchemical Accuracy. Journal of Chemical Theory and Computation, 2013, 9, 4287-4292.	2.3	88
20	Theoretical studies of RNA catalysis: Hybrid QM/MM methods and their comparison with MD and QM. Methods, 2009, 49, 202-216.	1.9	82
21	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.	1.3	79
22	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.	1.3	76
23	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.	2.3	67
24	Mechanical properties of symmetric and asymmetric DNA A-tracts: implications for looping and nucleosome positioning. Nucleic Acids Research, 2014, 42, 7383-7394.	6.5	59
25	How to understand atomistic molecular dynamics simulations of <scp>RNA</scp> and proteinâ€“<scp>RNA</scp> complexes?. Wiley Interdisciplinary Reviews RNA, 2017, 8, e1405.	3.2	54
26	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.	2.3	51
27	Extensions and applications of the A24 data set of accurate interaction energies. Physical Chemistry Chemical Physics, 2015, 17, 19268-19277.	1.3	50
28	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.	2.3	47
29	Quantum Monte Carlo for noncovalent interactions: an efficient protocol attaining benchmark accuracy. Physical Chemistry Chemical Physics, 2014, 16, 20915-20923.	1.3	46
30	How to understand quantum chemical computations on DNA and RNA systems? A practical guide for non-specialists. Methods, 2013, 64, 3-11.	1.9	45
31	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.	1.2	45
32	Lipid Enhanced Exfoliation for Production of Graphene Nanosheets. Journal of Physical Chemistry C, 2013, 117, 11800-11803.	1.5	38
33	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.	2.5	31
34	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.	2.3	30
35	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.	2.3	27
36	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.	2.3	27

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37	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.	1.2	27
38	Mechanical Model of DNA Allostery. Journal of Physical Chemistry Letters, 2014, 5, 3831-3835.	2.1	24
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.	2.3	24
40	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.	2.3	22
41	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.	1.2	20
42	Transferability and additivity of dihedral parameters in polarizable and nonpolarizable empirical force fields. Journal of Computational Chemistry, 2015, 36, 1874-1884.	1.5	15
43	On the Use of Molecular Dynamics Simulations for Probing Allostery through DNA. Biophysical Journal, 2016, 110, 874-876.	0.2	14
44	Toward Accurate Hydrogen Bonds by Scalable Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2019, 15, 3552-3557.	2.3	12
45	Conformational energies and equilibria of cyclic dinucleotidesin vacuoand in solution: computational chemistryvs.NMR experiments. Physical Chemistry Chemical Physics, 2021, 23, 7280-7294.	1.3	5
46	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.	1.5	5
47	Mapping the Chemical Space of the RNA Cleavage and Its Implications for Ribozyme Catalysis. Journal of Physical Chemistry B, 2017, 121, 10828-10840.	1.2	4