Rustam Z Khaliullin

List of Publications by Year
in descending order

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44 papers	9,104 citations	257357 24 h-index	265120 42 g-index
44 all docs	44 docs citations	44 times ranked	9928 citing authors

#	Article	IF	Citations
1	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	1.3	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
3	CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194103.	1.2	1,371
4	Unravelling the Origin of Intermolecular Interactions Using Absolutely Localized Molecular Orbitals. Journal of Physical Chemistry A, 2007, 111, 8753-8765.	1.1	508
5	Nucleation mechanism for the direct graphite-to-diamond phase transition. Nature Materials, 2011, 10, 693-697.	13.3	277
6	Analysis of charge transfer effects in molecular complexes based on absolutely localized molecular orbitals. Journal of Chemical Physics, 2008, 128, 184112.	1.2	188
7	An efficient self-consistent field method for large systems of weakly interacting components. Journal of Chemical Physics, 2006, 124, 204105.	1.2	179
8	Electronic signature of the instantaneous asymmetry in the first coordination shell of liquid water. Nature Communications, 2013, 4, 1450.	5.8	176
9	Electron Donation in the Waterâ€“Water Hydrogen Bond. Chemistry - A European Journal, 2009, 15, 851-855.	1.7	135
10	Ab initioquality neural-network potential for sodium. Physical Review B, 2010, 81, .	1.1	115
11	Graphite-diamond phase coexistence study employing a neural-network mapping of theab initiopotential energy surface. Physical Review B, 2010, 81, .	1.1	100
12	A Density Functional Theory Study of the Oxidation of Methanol to Formaldehyde over Vanadia Supported on Silica, Titania, and Zirconia. Journal of Physical Chemistry B, 2002, 106, 7832-7838.	1.2	98
13	A Density Functional Theory Study of the Mechanism of Free Radical Generation in the System Vanadate/PCA/H2O2. Journal of Physical Chemistry B, 2005, 109, 17984-17992.	1.2	85
14	Theoretical study of the rhenium alkane interaction in transition metal alkane Â-complexes. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 6963-6968.	3.3	73
15	Microscopic Origins of the Anomalous Melting Behavior of Sodium under High Pressure. Physical Review Letters, 2012, 108, 115701.	2.9	64
16	Nature of the Asymmetry in the Hydrogen-Bond Networks of Hexagonal Ice and Liquid Water. Journal of the American Chemical Society, 2014, 136, 3395-3399.	6.6	64
17	Covalency of hydrogen bonds in liquid water can be probed by proton nuclear magnetic resonance experiments. Nature Communications, 2015, 6, 8318.	5.8	61
18	Microscopic properties of liquid water from combined ab initio molecular dynamics and energy decomposition studies. Physical Chemistry Chemical Physics, 2013, 15, 15746.	1.3	55

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19	Interaction of Molecular Hydrogen with Open Transition Metal Centers for Enhanced Binding in Metal-Organic Frameworks: A Computational Study. Inorganic Chemistry, 2008, 47, 4032-4044.	1.9	48
20	Vibrational Signature of Water Molecules in Asymmetric Hydrogen Bonding Environments. Journal of Physical Chemistry Letters, 2013, 4, 3245-3250.	2.1	46
21	An Experimental and Density Functional Theory Study of the Interactions of CH4with Hâ^'ZSM-5. Journal of Physical Chemistry A, 2001, 105, 10454-10461.	1.1	42
22	Light-enabled metal-free pinacol coupling by hydrazine. Chemical Science, 2019, 10, 10937-10943.	3.7	33
23	Efficient Linear-Scaling Density Functional Theory for Molecular Systems. Journal of Chemical Theory and Computation, 2013, 9, 4421-4427.	2.3	28
24	On the role of interfacial hydrogen bonds in â€œon-waterâ€•catalysis. Journal of Chemical Physics, 2014, 141, 22D528.	1.2	26
25	Photocatalytic Methylation of Nonactivated sp³ and sp² Câ€“H Bonds Using Methanol on GaN. ACS Catalysis, 2020, 10, 6248-6253.	5.5	21
26	Direct deoxygenative borylation of carboxylic acids. Nature Communications, 2021, 12, 4970.	5.8	20
27	Empowering alcohols as carbonyl surrogates for Grignard-type reactions. Nature Communications, 2020, 11, 6022.	5.8	14
28	Energy Decomposition Analysis for Metal Surfaceâ€“Adsorbate Interactions by Block Localized Wave Functions. Journal of Chemical Theory and Computation, 2019, 15, 265-275.	2.3	13
29	Low-Dimensional Confined Ice Has the Electronic Signature of Liquid Water. Journal of Physical Chemistry Letters, 2019, 10, 2008-2016.	2.1	11
30	Stereospecific Epitaxial Growth of Bilayered Porous Molecular Networks. Journal of the American Chemical Society, 2020, 142, 8662-8671.	6.6	11
31	Adatoms in the Surface-Confined Ullmann Coupling of Phenyl Groups. Journal of Physical Chemistry Letters, 2021, 12, 11061-11069.	2.1	11
32	Theoretical Study of Solvent Effects on the Thermodynamics of Iron(III) [Tetrakis(pentafluorophenyl)]porphyrin Chloride Dissociation. Journal of Physical Chemistry B, 2007, 111, 10992-10998.	1.2	10
33	Redox-Triggered Disassembly of Nanosized Liposomes Containing Ferrocene-Appended Amphiphiles. Langmuir, 2019, 35, 5608-5616.	1.6	9
34	On the Possibility of Helium Adsorption in Nitrogen Doped Graphitic Materials. Scientific Reports, 2020, 10, 5832.	1.6	9
35	Unraveling the Origins of Strong and Reversible Chemisorption of Carbon Dioxide in a Green Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2021, 125, 24719-24727.	1.5	9
36	Light-driven transition-metal-free direct decarbonylation of unstrained diaryl ketones via a dual Câ€“C bond cleavage. Nature Communications, 2022, 13, 1805.	5.8	9

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37	Contribution of the Covalent Component of the Hydrogen-Bond Network to the Properties of Liquid Water. Journal of Physical Chemistry A, 2018, 122, 7482-7490.	1.1	8
38	Communication: Compact orbitals enable low-cost linear-scaling ab initio molecular dynamics for weakly-interacting systems. Journal of Chemical Physics, 2018, 148, 231103.	1.2	6
39	Why pregnenolone and progesterone, two structurally similar steroids, exhibit remarkably different cocrystallization with aromatic molecules. Physical Chemistry Chemical Physics, 2018, 20, 898-904.	1.3	5
40	Correlated Local Fluctuations in the Hydrogen Bond Network of Liquid Water. Journal of the American Chemical Society, 2022, 144, 13127-13136.	6.6	4
41	Tetraedrisch, wenn flÃ¼ssig. Nachrichten Aus Der Chemie, 2013, 61, 1203-1206.	0.0	2
42	Direct Unconstrained Variable-Metric Localization of One-Electron Orbitals. Journal of Chemical Theory and Computation, 2020, 16, 3558-3566.	2.3	2
43	Efficient evaluation of the error vector in the direct inversion in the iterative subspace scheme. Chemical Physics Letters, 2006, 418, 359-360.	1.2	0
44	Variable-Metric Localization of Occupied and Virtual Orbitals. Journal of Chemical Theory and Computation, 2021, 17, 5568-5581.	2.3	0