Rustam Z Khaliullin

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6737401/publications.pdf

Version: 2024-02-01

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	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
2	Correlated Local Fluctuations in the Hydrogen Bond Network of Liquid Water. Journal of the American Chemical Society, 2022, 144, 13127-13136.	6.6	4
3	Direct deoxygenative borylation of carboxylic acids. Nature Communications, 2021, 12, 4970.	5.8	20
4	Variable-Metric Localization of Occupied and Virtual Orbitals. Journal of Chemical Theory and Computation, 2021, 17, 5568-5581.	2.3	0
5	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
6	Adatoms in the Surface-Confined Ullmann Coupling of Phenyl Groups. Journal of Physical Chemistry Letters, 2021, 12, 11061-11069.	2.1	11
7	On the Possibility of Helium Adsorption in Nitrogen Doped Graphitic Materials. Scientific Reports, 2020, 10, 5832.	1.6	9
8	Empowering alcohols as carbonyl surrogates for Grignard-type reactions. Nature Communications, 2020, 11, 6022.	5.8	14
9	Photocatalytic Methylation of Nonactivated sp³ and sp² Câ€“H Bonds Using Methanol on GaN. ACS Catalysis, 2020, 10, 6248-6253.	5.5	21
10	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
11	Direct Unconstrained Variable-Metric Localization of One-Electron Orbitals. Journal of Chemical Theory and Computation, 2020, 16, 3558-3566.	2.3	2
12	Stereospecific Epitaxial Growth of Bilayered Porous Molecular Networks. Journal of the American Chemical Society, 2020, 142, 8662-8671.	6.6	11
13	Light-enabled metal-free pinacol coupling by hydrazine. Chemical Science, 2019, 10, 10937-10943.	3.7	33
14	Redox-Triggered Disassembly of Nanosized Liposomes Containing Ferrocene-Appended Amphiphiles. Langmuir, 2019, 35, 5608-5616.	1.6	9
15	Low-Dimensional Confined Ice Has the Electronic Signature of Liquid Water. Journal of Physical Chemistry Letters, 2019, 10, 2008-2016.	2.1	11
16	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
17	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
18	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

#	Article	IF	Citations
19	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
20	Covalency of hydrogen bonds in liquid water can be probed by proton nuclear magnetic resonance experiments. Nature Communications, 2015, 6, 8318.	5.8	61
21	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
22	On the role of interfacial hydrogen bonds in â€œon-waterâ€•catalysis. Journal of Chemical Physics, 2014, 141, 22D528.	1.2	26
23	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
24	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
25	Vibrational Signature of Water Molecules in Asymmetric Hydrogen Bonding Environments. Journal of Physical Chemistry Letters, 2013, 4, 3245-3250.	2.1	46
26	Efficient Linear-Scaling Density Functional Theory for Molecular Systems. Journal of Chemical Theory and Computation, 2013, 9, 4421-4427.	2.3	28
27	Electronic signature of the instantaneous asymmetry in the first coordination shell of liquid water. Nature Communications, 2013, 4, 1450.	5.8	176
28	Tetraedrisch, wenn flÃ¼ssig. Nachrichten Aus Der Chemie, 2013, 61, 1203-1206.	0.0	2
29	Microscopic Origins of the Anomalous Melting Behavior of Sodium under High Pressure. Physical Review Letters, 2012, 108, 115701.	2.9	64
30	Nucleation mechanism for the direct graphite-to-diamond phase transition. Nature Materials, 2011, 10, 693-697.	13.3	277
31	Ab initioquality neural-network potential for sodium. Physical Review B, 2010, 81, .	1.1	115
32	Graphite-diamond phase coexistence study employing a neural-network mapping of theab initiopotential energy surface. Physical Review B, 2010, 81, .	1.1	100
33	Electron Donation in the Waterâ€“Water Hydrogen Bond. Chemistry - A European Journal, 2009, 15, 851-855.	1.7	135
34	Analysis of charge transfer effects in molecular complexes based on absolutely localized molecular orbitals. Journal of Chemical Physics, 2008, 128, 184112.	1.2	188
35	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
36	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

#	Article	IF	Citations
37	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
38	Unravelling the Origin of Intermolecular Interactions Using Absolutely Localized Molecular Orbitals. Journal of Physical Chemistry A, 2007, 111, 8753-8765.	1.1	508
39	An efficient self-consistent field method for large systems of weakly interacting components. Journal of Chemical Physics, 2006, 124, 204105.	1.2	179
40	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
41	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	1.3	2,597
42	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
43	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
44	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