

Raimondas Galvelis

List of Publications by Year in descending order

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Version: 2024-02-01

16
papers

1,228
citations

759233

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1125743

13
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all docs

18
docs citations

18
times ranked

1763
citing authors

#	ARTICLE	IF	CITATIONS
1	P<sc>SI4</sc> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	3.0	440
2	A Scalable Molecular Force Field Parameterization Method Based on Density Functional Theory and Quantum-Level Machine Learning. Journal of Chemical Information and Modeling, 2019, 59, 3485-3493.	5.4	52
3	Enhanced Conformational Sampling of N-Glycans in Solution with Replica State Exchange Metadynamics. Journal of Chemical Theory and Computation, 2017, 13, 1934-1942.	5.3	16
4	Neural Network and Nearest Neighbor Algorithms for Enhancing Sampling of Molecular Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 2489-2500.	5.3	51
5	Replica State Exchange Metadynamics for Improving the Convergence of Free Energy Estimates. Journal of Computational Chemistry, 2016, 37, .	3.3	0
6	Exploring N-Glycan Conformers: Assessment of Enhanced Sampling Algorithms. Biophysical Journal, 2016, 110, 643a.	0.5	0
7	Coarse graining of force fields for metal-organic frameworks. Dalton Transactions, 2016, 45, 4370-4379.	3.3	32
8	Computational Approaches to the Design, Crystal Structure Prediction, and Structure-Property Relationships of Metal-Organic Frameworks. , 2015, , 1-52.		0
9	Replica state exchange metadynamics for improving the convergence of free energy estimates. Journal of Computational Chemistry, 2015, 36, 1446-1455.	3.3	18
10	Impact of functionalized linkers on the energy landscape of ZIFs. CrystEngComm, 2013, 15, 9603.	2.6	28
11	Exceptionally Low Shear Modulus in a Prototypical Imidazole-Based Metal-Organic Framework. Physical Review Letters, 2012, 108, 095502.	7.8	210
12	Flexibility and swing effect on the adsorption of energy-related gases on ZIF-8: combined experimental and simulation study. Dalton Transactions, 2012, 41, 10752.	3.3	176
13	Prediction on the existence and chemical stability of cuprous fluoride. Chemical Science, 2012, 3, 2565.	7.4	22
14	Comparison of the relative stability of zinc and lithium-boron zeolitic imidazolate frameworks. CrystEngComm, 2012, 14, 374-378.	2.6	47
15	Mechanical Properties of Dense Zeolitic Imidazolate Frameworks (ZIFs): A High-Pressure X-ray Diffraction, Nanoindentation and Computational Study of the Zinc Framework Zn(Im) ₂ , and its Lithium-Boron Analogue, LiB(Im) ₄ . Chemistry - A European Journal, 2010, 16, 10684-10690.	3.3	119
16	Deposition of BaHfO ₃ Dielectric Layers for Microelectronic Applications by Pulsed Liquid Injection MOCVD. Chemical Vapor Deposition, 2009, 15, 167-170.	1.3	5