Raimondas Galvelis

List of Publications by Year
in descending order

16	1,228	759233 12	1125743 13
papers	citations	h-index	g-index

18	18	18	1763
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	3.0	440
2	Exceptionally Low Shear Modulus in a Prototypical Imidazole-Based Metal-Organic Framework. Physical Review Letters, 2012, 108, 095502.	7.8	210
3	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
4	Mechanical Properties of Dense Zeolitic Imidazolate Frameworks (ZIFs): A Highâ€Pressure Xâ€ray Diffraction, Nanoindentation and Computational Study of the Zinc Framework Zn(Im)₂, and its Lithiumï£¿Boron Analogue, LiB(Im)₄. Chemistry - A European Journal, 2010, 16, 10684-10690.	3.3	119
5	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
6	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
7	Comparison of the relative stability of zinc and lithium-boron zeolitic imidazolate frameworks. CrystEngComm, 2012, 14, 374-378.	2.6	47
8	Coarse graining of force fields for metalâ€“organic frameworks. Dalton Transactions, 2016, 45, 4370-4379.	3.3	32
9	Impact of functionalized linkers on the energy landscape of ZIFs. CrystEngComm, 2013, 15, 9603.	2.6	28
10	Prediction on the existence and chemical stability of cuprous fluoride. Chemical Science, 2012, 3, 2565.	7.4	22
11	Replica state exchange metadynamics for improving the convergence of free energy estimates. Journal of Computational Chemistry, 2015, 36, 1446-1455.	3.3	18
12	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
13	Deposition of BaHfO₃ Dielectric Layers for Microelectronic Applications by Pulsed Liquid Injection MOCVD. Chemical Vapor Deposition, 2009, 15, 167-170.	1.3	5
14	Computational Approaches to the Design, Crystal Structure Prediction, and Structureâ€“Property Relationships of Metalâ€“Organic Frameworks. , 2015, , 1-52.		0
15	Replica State Exchange Metadynamics for Improving the Convergence of Free Energy Estimates. Journal of Computational Chemistry, 2016, 37, .	3.3	0
16	Exploring N-Glycan Conformers: Assessment of Enhanced Sampling Algorithms. Biophysical Journal, 2016, 110, 643a.	0.5	0