Guido Falk von Rudorff

List of Publications by Year
in descending order

26	505	623734 14	677142 22
papers	citations	h-index	g-index

26	26	26	666
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Evaluating quantum alchemy of atoms with thermodynamic cycles: Beyond ground electronic states. Journal of Chemical Physics, 2022, 156, 064106.	3.0	5
2	Quantum alchemy beyond singlets: Bonding in diatomic molecules with hydrogen. Journal of Chemical Physics, 2022, 156, .	3.0	2
3	Ab initio machine learning of phase space averages. Journal of Chemical Physics, 2022, 157, .	3.0	4
4	Simplifying inverse materials design problems for fixed lattices with alchemical chirality. Science Advances, 2021, 7, .	10.3	6
5	Elucidating an Atmospheric Brown Carbon Speciesâ€”Toward Supplanting Chemical Intuition with Exhaustive Enumeration and Machine Learning. Environmental Science & Technology, 2021, 55, 8447-8457.	10.0	6
6	Machine learning based energy-free structure predictions of molecules, transition states, and solids. Nature Communications, 2021, 12, 4468.	12.8	53
7	Toward the design of chemical reactions: Machine learning barriers of competing mechanisms in reactant space. Journal of Chemical Physics, 2021, 155, 064105.	3.0	37
8	Arbitrarily accurate quantum alchemy. Journal of Chemical Physics, 2021, 155, 224103.	3.0	9
9	Rapid and accurate molecular deprotonation energies from quantum alchemy. Physical Chemistry Chemical Physics, 2020, 22, 10519-10525.	2.8	19
10	Data enhanced Hammett-equation: reaction barriers in chemical space. Chemical Science, 2020, 11, 11859-11868.	7.4	29
11	Effects of perturbation order and basis set on alchemical predictions. Journal of Chemical Physics, 2020, 153, 144118.	3.0	14
12	Machine learning the computational cost of quantum chemistry. Machine Learning: Science and Technology, 2020, 1, 025002.	5.0	25
13	Thousands of reactants and transition states for competing E2 and S N 2 reactions. Machine Learning: Science and Technology, 2020, 1, 045026.	5.0	33
14	Alchemical perturbation density functional theory. Physical Review Research, 2020, 2, .	3.6	23
15	Atoms in Molecules from Alchemical Perturbation Density Functional Theory. Journal of Physical Chemistry B, 2019, 123, 10073-10082.	2.6	18
16	Acidity Constants of the Hematiteâ€“Liquid Water Interface from Ab Initio Molecular Dynamics. Journal of Physical Chemistry Letters, 2018, 9, 5574-5582.	4.6	25
17	Conformational Space of a Polyphilic Molecule with a Fluorophilic Side Chain Integrated in a DPPC Bilayer. Journal of Computational Chemistry, 2017, 38, 576-583.	3.3	4
18	Dynamic Stabilization of Metal Oxideâ€“Water Interfaces. Journal of the American Chemical Society, 2017, 139, 2581-2584.	13.7	60

#	Article	IF	Citations
19	Improving the Performance of Hybrid Functional-Based Molecular Dynamics Simulation through Screening of Hartreeâ€“Fock Exchange Forces. Journal of Chemical Theory and Computation, 2017, 13, 2178-2184.	5.3	9
20	Cysteine Linkages Accelerate Electron Flow through Tetra-Heme Protein STC. Journal of the American Chemical Society, 2017, 139, 17237-17240.	13.7	40
21	Cluster Formation of Polyphilic Molecules Solvated in a DPPC Bilayer. Polymers, 2017, 9, 488.	4.5	1
22	Hematite(001)-liquid water interface from hybrid density functional-based molecular dynamics. Journal of Physics Condensed Matter, 2016, 28, 394001.	1.8	20
23	Fast Interconversion of Hydrogen Bonding at the Hematite (001)â€“Liquid Water Interface. Journal of Physical Chemistry Letters, 2016, 7, 1155-1160.	4.6	42
24	Efficient implementation and application of the artificial bee colony algorithm to low-dimensional optimization problems. Computer Physics Communications, 2014, 185, 1639-1646.	7.5	3
25	Perfluoroalkane Force Field for Lipid Membrane Environments. Journal of Physical Chemistry B, 2014, 118, 12531-12540.	2.6	10
26	Foraging on the potential energy surface: A swarm intelligence-based optimizer for molecular geometry. Journal of Chemical Physics, 2012, 137, 194110.	3.0	8