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	Dynamic Stabilization of Metal Oxideâ€“Water Interfaces. Journal of the American Chemical Society, 2017, 139, 2581-2584.	13.7	60
2	Machine learning based energy-free structure predictions of molecules, transition states, and solids. Nature Communications, 2021, 12, 4468.	12.8	53
3	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
4	Cysteine Linkages Accelerate Electron Flow through Tetra-Heme Protein STC. Journal of the American Chemical Society, 2017, 139, 17237-17240.	13.7	40
5	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
6	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
7	Data enhanced Hammett-equation: reaction barriers in chemical space. Chemical Science, 2020, 11, 11859-11868.	7.4	29
8	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
9	Machine learning the computational cost of quantum chemistry. Machine Learning: Science and Technology, 2020, 1, 025002.	5.0	25
10	Alchemical perturbation density functional theory. Physical Review Research, 2020, 2, .	3.6	23
11	Hematite(001)-liquid water interface from hybrid density functional-based molecular dynamics. Journal of Physics Condensed Matter, 2016, 28, 394001.	1.8	20
12	Rapid and accurate molecular deprotonation energies from quantum alchemy. Physical Chemistry Chemical Physics, 2020, 22, 10519-10525.	2.8	19
13	Atoms in Molecules from Alchemical Perturbation Density Functional Theory. Journal of Physical Chemistry B, 2019, 123, 10073-10082.	2.6	18
14	Effects of perturbation order and basis set on alchemical predictions. Journal of Chemical Physics, 2020, 153, 144118.	3.0	14
15	Perfluoroalkane Force Field for Lipid Membrane Environments. Journal of Physical Chemistry B, 2014, 118, 12531-12540.	2.6	10
16	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
17	Arbitrarily accurate quantum alchemy. Journal of Chemical Physics, 2021, 155, 224103.	3.0	9
18	Foraging on the potential energy surface: A swarm intelligence-based optimizer for molecular geometry. Journal of Chemical Physics, 2012, 137, 194110.	3.0	8

#	Article	IF	Citations
19	Simplifying inverse materials design problems for fixed lattices with alchemical chirality. Science Advances, 2021, 7, .	10.3	6
20	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
21	Evaluating quantum alchemy of atoms with thermodynamic cycles: Beyond ground electronic states. Journal of Chemical Physics, 2022, 156, 064106.	3.0	5
22	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
23	Ab initio machine learning of phase space averages. Journal of Chemical Physics, 2022, 157, .	3.0	4
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	Quantum alchemy beyond singlets: Bonding in diatomic molecules with hydrogen. Journal of Chemical Physics, 2022, 156, .	3.0	2
26	Cluster Formation of Polyphilic Molecules Solvated in a DPPC Bilayer. Polymers, 2017, 9, 488.	4.5	1