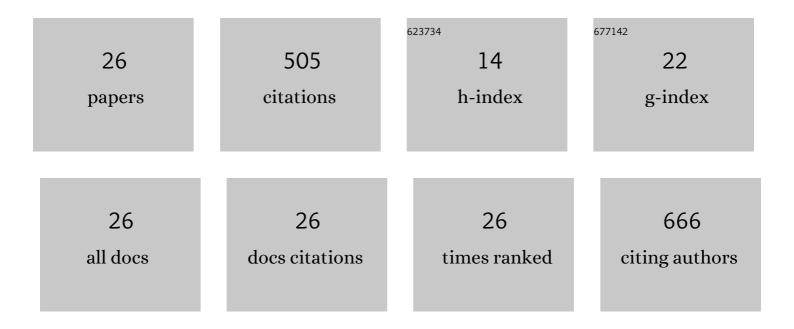
## Guido Falk von Rudorff

List of Publications by Year in descending order

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#	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	<i>Ab initio</i> 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 Species—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 Hematite–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 Oxide–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 Hartree–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)–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