Leslie Vogt

List of Publications by Year
in descending order

32 papers	6,690 citations	257450 24 h-index	414414 32 g-index
35 all docs	35 docs citations	35 times ranked	8803 citing authors

#	Article	IF	Citations
1	Crystal Structure Predictions for 4-Amino-2,3,6-trinitrophenol Using a Tailor-Made First-Principles-Based Force Field. Crystal Growth and Design, 2022, 22, 1182-1195.	3.0	3
2	Non-Monotonic Temperature Dependence of Hydroxide Ion Diffusion in Anion Exchange Membranes. Chemistry of Materials, 2022, 34, 2133-2145.	6.7	25
3	Insights into the Polymorphic Structures and Enantiotropic Layer-Slip Transition in Paracetamol Form III from Enhanced Molecular Dynamics. Crystal Growth and Design, 2021, 21, 886-896.	3.0	8
4	Imidacloprid Crystal Polymorphs for Disease Vector Control and Pollinator Protection. Journal of the American Chemical Society, 2021, 143, 17144-17152.	13.7	27
5	Quantum chemical accuracy from density functional approximations via machine learning. Nature Communications, 2020, 11, 5223.	12.8	187
6	Generating Cocrystal Polymorphs with Information Entropy Driven by Molecular Dynamics-Based Enhanced Sampling. Journal of Physical Chemistry Letters, 2020, 11, 9751-9758.	4.6	10
7	Disorderly Conduct of Benzamide IV: Crystallographic and Computational Analysis of High Entropy Polymorphs of Small Molecules. Crystal Growth and Design, 2020, 20, 2670-2682.	3.0	18
8	Why Are Some Crystals Straight?. Journal of Physical Chemistry C, 2020, 124, 15616-15624.	3.1	26
9	Hydroxide Ion Diffusion in Anion-Exchange Membranes at Low Hydration: Insights from Ab Initio Molecular Dynamics. Chemistry of Materials, 2019, 31, 5778-5787.	6.7	64
10	Melt Crystallization for Paracetamol Polymorphism. Crystal Growth and Design, 2019, 19, 4070-4080.	3.0	64
11	Machine learning and the physical sciences. Reviews of Modern Physics, 2019, 91, .	45.6	1,245
12	Endpoint-restricted adiabatic free energy dynamics approach for the exploration of biomolecular conformational equilibria. Journal of Chemical Physics, 2018, 149, 072316.	3.0	11
13	Powder diffraction and crystal structure prediction identify four new coumarin polymorphs. Chemical Science, 2017, 8, 4926-4940.	7.4	97
14	Bypassing the Kohn-Sham equations with machine learning. Nature Communications, 2017, 8, 872.	12.8	485
15	Exploring polymorphism of benzene and naphthalene with free energy based enhanced molecular dynamics. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 542-550.	1.1	41
16	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	1.1	445
17	Isostructural Cocrystals of 1,3,5-Trinitrobenzene Assembled by Halogen Bonding. Crystal Growth and Design, 2016, 16, 4688-4693.	3.0	47
18	Oxygen-evolving complex of Photosystem II: an analysis of second-shell residues and hydrogen-bonding networks. Current Opinion in Chemical Biology, 2015, 25, 152-158.	6.1	102

#	Article	IF	Citations
19	Computational Insights on Crystal Structures of the Oxygen-Evolving Complex of Photosystem II with Either Ca²⁺ or Ca²⁺ Substituted by Sr²⁺. Biochemistry, 2015, 54, 820-825.	2.5	31
20	Proton-Coupled Electron Transfer During the S-State Transitions of the Oxygen-Evolving Complex of Photosystem II. Journal of Physical Chemistry B, 2015, 119, 7366-7377.	2.6	49
21	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
22	Single Molecule Rectification Induced by the Asymmetry of a Single Frontier Orbital. Journal of Chemical Theory and Computation, 2014, 10, 3393-3400.	5.3	36
23	High-Conductance Conformers in Histograms of Single-Molecule Currentâ€“Voltage Characteristics. Journal of Physical Chemistry C, 2014, 118, 8316-8321.	3.1	12
24	S₀-State Model of the Oxygen-Evolving Complex of Photosystem II. Biochemistry, 2013, 52, 7703-7706.	2.5	97
25	Electrostatic Effects on Proton Coupled Electron Transfer in Oxomanganese Complexes Inspired by the Oxygen-Evolving Complex of Photosystem II. Journal of Physical Chemistry B, 2013, 117, 6217-6226.	2.6	36
26	Accelerated computational discovery of high-performance materials for organic photovoltaics by means of cheminformatics. Energy and Environmental Science, 2011, 4, 4849.	30.8	169
27	The Harvard Clean Energy Project: Large-Scale Computational Screening and Design of Organic Photovoltaics on the World Community Grid. Journal of Physical Chemistry Letters, 2011, 2, 2241-2251.	4.6	470
28	Accelerating Correlated Quantum Chemistry Calculations Using Graphical Processing Units and a Mixed Precision Matrix Multiplication Library. Journal of Chemical Theory and Computation, 2010, 6, 135-144.	5.3	75
29	Engineering directed excitonic energy transfer. Applied Physics Letters, 2010, 96, 093114.	3.3	33
30	Examination of pigments on Thai manuscripts: the first identification of copper citrate. Journal of Raman Spectroscopy, 2008, 39, 1057-1065.	2.5	26
31	Accelerating Resolution-of-the-Identity Second-Order MÃ¸llerâ€“Plesset Quantum Chemistry Calculations with Graphical Processing Units. Journal of Physical Chemistry A, 2008, 112, 2049-2057.	2.5	133
32	Automated compound classification for ambient aerosol sample separations using comprehensive two-dimensional gas chromatographyâ€“time-of-flight mass spectrometry. Journal of Chromatography A, 2007, 1150, 2-12.	3.7	51