# Leslie Vogt

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215. | 1.7 | 2,561 |
| 2 | Machine learning and the physical sciences. Reviews of Modern Physics, 2019, 91, . | 45.6 | 1,245 |
| 3 | Bypassing the Kohn-Sham equations with machine learning. Nature Communications, 2017, 8, 872. | 12.8 | 485 |
| 4 | 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 |
| 5 | 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 |
| 6 | Quantum chemical accuracy from density functional approximations via machine learning. Nature Communications, 2020, 11, 5223. | 12.8 | 187 |
| 7 | Accelerated computational discovery of high-performance materials for organic photovoltaics by means of cheminformatics. Energy and Environmental Science, 2011, 4, 4849. | 30.8 | 169 |
| 8 | 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 |
| 9 | 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 |
| 10 | S<sub>0</sub>-State Model of the Oxygen-Evolving Complex of Photosystem II. Biochemistry, 2013, 52, 7703-7706. | 2.5 | 97 |
| 11 | Powder diffraction and crystal structure prediction identify four new coumarin polymorphs. Chemical Science, 2017, 8, 4926-4940. | 7.4 | 97 |
| 12 | 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 |
| 13 | 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 |
| 14 | Melt Crystallization for Paracetamol Polymorphism. Crystal Growth and Design, 2019, 19, 4070-4080. | 3.0 | 64 |
| 15 | 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 |
| 16 | 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 |
| 17 | Isostructural Cocrystals of 1,3,5-Trinitrobenzene Assembled by Halogen Bonding. Crystal Growth and Design, 2016, 16, 4688-4693. | 3.0 | 47 |
| 18 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | 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 |
| 21 | Engineering directed excitonic energy transfer. Applied Physics Letters, 2010, 96, 093114. | 3.3 | 33 |
| 22 | Computational Insights on Crystal Structures of the Oxygen-Evolving Complex of Photosystem II with Either Ca<sup>2+</sup> or Ca<sup>2+</sup> Substituted by Sr<sup>2+</sup>. Biochemistry, 2015, 54, 820-825. | 2.5 | 31 |
| 23 | Imidacloprid Crystal Polymorphs for Disease Vector Control and Pollinator Protection. Journal of the American Chemical Society, 2021, 143, 17144-17152. | 13.7 | 27 |
| 24 | Examination of pigments on Thai manuscripts: the first identification of copper citrate. Journal of Raman Spectroscopy, 2008, 39, 1057-1065. | 2.5 | 26 |
| 25 | Why Are Some Crystals Straight?. Journal of Physical Chemistry C, 2020, 124, 15616-15624. | 3.1 | 26 |
| 26 | Non-Monotonic Temperature Dependence of Hydroxide Ion Diffusion in Anion Exchange Membranes. Chemistry of Materials, 2022, 34, 2133-2145. | 6.7 | 25 |
| 27 | 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 |
| 28 | High-Conductance Conformers in Histograms of Single-Molecule Currentâ€“Voltage Characteristics. Journal of Physical Chemistry C, 2014, 118, 8316-8321. | 3.1 | 12 |
| 29 | Endpoint-restricted adiabatic free energy dynamics approach for the exploration of biomolecular conformational equilibria. Journal of Chemical Physics, 2018, 149, 072316. | 3.0 | 11 |
| 30 | 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 |
| 31 | 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 |
| 32 | 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 |