Alexander Urban

List of Publications by Year
in descending order

39 papers	5,183 citations	236925 25 h-index	315739 38 g-index
39 all docs	39 docs citations	39 times ranked	5489 citing authors

#	Article	IF	Citations
1	The structural and chemical origin of the oxygen redox activity in layered and cation-disordered Li-excess cathode materials. Nature Chemistry, 2016, 8, 692-697.	13.6	1,022
2	Unlocking the Potential of Cation-Disordered Oxides for Rechargeable Lithium Batteries. Science, 2014, 343, 519-522.	12.6	943
3	Computational understanding of Li-ion batteries. Npj Computational Materials, 2016, 2, .	8.7	411
4	An implementation of artificial neural-network potentials for atomistic materials simulations: Performance for TiO2. Computational Materials Science, 2016, 114, 135-150.	3.0	377
5	The Configurational Space of Rocksaltâ€Type Oxides for Highâ€Capacity Lithium Battery Electrodes. Advanced Energy Materials, 2014, 4, 1400478.	19.5	256
6	Efficient and accurate machine-learning interpolation of atomic energies in compositions with many species. Physical Review B, 2017, 96, .	3.2	228
7	Hidden structural and chemical order controls lithium transport in cation-disordered oxides for rechargeable batteries. Nature Communications, 2019, 10, 592.	12.8	162
8	Ultrahigh power and energy density in partially ordered lithium-ion cathode materials. Nature Energy, 2020, 5, 213-221.	39.5	158
9	A disordered rock-salt Li-excess cathode material with high capacity and substantial oxygen redox activity: Li 1.25 Nb 0.25 Mn 0.5 O 2. Electrochemistry Communications, 2015, 60, 70-73.	4.7	145
10	Electronic-Structure Origin of Cation Disorder in Transition-Metal Oxides. Physical Review Letters, 2017, 119, 176402.	7.8	135
11	The Intercalation Phase Diagram of Mg in V₂O₅ from First-Principles. Chemistry of Materials, 2015, 27, 3733-3742.	6.7	130
12	Calibrating transition-metal energy levels and oxygen bands in first-principles calculations: Accurate prediction of redox potentials and charge transfer in lithium transition-metal oxides. Physical Review B, 2015, 92, .	3.2	126
13	Constructing first-principles phase diagrams of amorphous LixSi using machine-learning-assisted sampling with an evolutionary algorithm. Journal of Chemical Physics, 2018, 148, 241711.	3.0	121
14	Stoichiometric Layered Potassium Transition Metal Oxide for Rechargeable Potassium Batteries. Chemistry of Materials, 2018, 30, 6532-6539.	6.7	108
15	Computational Design and Preparation of Cationâ€Disordered Oxides for Highâ€Energyâ€Density Liâ€Ion Batteries. Advanced Energy Materials, 2016, 6, 1600488.	19.5	93
16	Effect of Fluorination on Lithium Transport and Shortâ€Range Order in Disorderedâ€Rocksaltâ€Type Lithiumâ€Ion Battery Cathodes. Advanced Energy Materials, 2020, 10, 1903240.	19.5	83
17	Understanding the Effect of Cation Disorder on the Voltage Profile of Lithium Transition-Metal Oxides. Chemistry of Materials, 2016, 28, 5373-5383.	6.7	79
18	First-Principles Simulation of the (Liâ€“Niâ€“Vacancy)O Phase Diagram and Its Relevance for the Surface Phases in Ni-Rich Li-Ion Cathode Materials. Chemistry of Materials, 2017, 29, 7840-7851.	6.7	79

#	Article	IF	Citations
19	Influence of Inversion on Mg Mobility and Electrochemistry in Spinels. Chemistry of Materials, 2017, 29, 7918-7930.	6.7	75
20	The Effect of Cation Disorder on the Average Li Intercalation Voltage of Transition-Metal Oxides. Chemistry of Materials, 2016, 28, 3659-3665.	6.7	62
21	Designing New Lithium-Excess Cathode Materials from Percolation Theory: Nanohighways in Li_xNi_{2â€“4x/3}Sb_{x/3}O₂. Nano Letters, 2015, 15, 596-602.	9.1	54
22	Tuning the Reactivity of Oxide Surfaces by Chargeâ€Accepting Adsorbates. Angewandte Chemie - International Edition, 2007, 46, 7315-7318.	13.8	53
23	Strategies for the construction of machine-learning potentials for accurate and efficient atomic-scale simulations. Machine Learning: Science and Technology, 2021, 2, 031001.	5.0	42
24	Efficient training of ANN potentials by including atomic forces via Taylor expansion and application to water and a transition-metal oxide. Npj Computational Materials, 2020, 6, .	8.7	40
25	Realizing continuous cation order-to-disorder tuning in a class of high-energy spinel-type Li-ion cathodes. Matter, 2021, 4, 3897-3916.	10.0	32
26	Finding and proving the exact ground state of a generalized Ising model by convex optimization and MAX-SAT. Physical Review B, 2016, 94, .	3.2	25
27	Accelerated Atomistic Modeling of Solid-State Battery Materials With Machine Learning. Frontiers in Energy Research, 2021, 9, .	2.3	25
28	Effect of fluorination and Li-excess on the Li migration barrier in Mn-based cathode materials. Journal of Materials Chemistry A, 2020, 8, 19965-19974.	10.3	20
29	Stackingâ€Fault Enhanced Oxygen Redox in Li₂MnO₃. Advanced Energy Materials, 2022, 12, .	19.5	17
30	Growth of One-Dimensional Pd Nanowires on the Terraces of a ReducedSnO2(101)Surface. Physical Review Letters, 2007, 98, 186102.	7.8	16
31	Understanding the Origin of Higher Capacity for Ni-Based Disordered Rock-Salt Cathodes. Chemistry of Materials, 2020, 32, 3447-3461.	6.7	16
32	Construction of ground-state preserving sparse lattice models for predictive materials simulations. Npj Computational Materials, 2017, 3, .	8.7	15
33	Augmenting zero-Kelvin quantum mechanics with machine learning for the prediction of chemical reactions at high temperatures. Nature Communications, 2021, 12, 7012.	12.8	10
34	Understanding the Onset of Surface Degradation in LiNiO₂ Cathodes. ACS Applied Energy Materials, 2022, 5, 5730-5741.	5.1	10
35	Data-driven approach to parameterize <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>SCAN</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:m for an accurate description of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml: transition metal oxide thermochemistry. Physical Review Materials, 2022, 6, .	2.4	6
36	Anisotropic to Isotropic Transition in Monolayer Group-IV Tellurides. Materials, 2021, 14, 4495.	2.9	4

#	Article	IF	Citations
37	Electrodes: The Configurational Space of Rocksalt-Type Oxides for High-Capacity Lithium Battery Electrodes (Adv. Energy Mater. 13/2014). Advanced Energy Materials, 2014, 4, n/a-n/a.	19.5	3
38	Potential and pH Dependence of the Buried Interface of Membrane-Coated Electrocatalysts. ACS Applied Materials & Interfaces, 2020, 12, 52125-52135.	8.0	2
39	Lithium Batteries: Computational Design and Preparation of Cation-Disordered Oxides for High-Energy-Density Li-Ion Batteries (Adv. Energy Mater. 15/2016). Advanced Energy Materials, 2016, 6, .	19.5	0