Ryan Jacobs

List of Publications by Year
in descending order

		394421	302126
41 papers	2,059 citations	19 h-index	39 g-index
42 all docs	42 docs citations	42 times ranked	3246 citing authors

#	Article	IF	Citations
1	Electronic Structure-Based Descriptors for Oxide Properties and Functions. Accounts of Chemical Research, 2022, 55, 298-308.	15.6	42
2	Machine learning for impurity charge-state transition levels in semiconductors from elemental properties using multi-fidelity datasets. Journal of Chemical Physics, 2022, 156, 114110.	3.0	5
3	Machine learning predictions of irradiation embrittlement in reactor pressure vessel steels. Npj Computational Materials, 2022, 8, .	8.7	9
4	Performance and limitations of deep learning semantic segmentation of multiple defects in transmission electron micrographs. Cell Reports Physical Science, 2022, 3, 100876.	5.6	10
5	Unconventional Highly Active and Stable Oxygen Reduction Catalysts Informed by Computational Design Strategies. Advanced Energy Materials, 2022, 12, .	19.5	4
6	Deep learning object detection in materials science: Current state and future directions. Computational Materials Science, 2022, 211, 111527.	3.0	20
7	Calibration after bootstrap for accurate uncertainty quantification in regression models. Npj Computational Materials, 2022, 8, .	8.7	15
8	Discovery and engineering of low work function perovskite materials. Journal of Materials Chemistry C, 2021, 9, 12778-12790.	5.5	15
9	Work Function Trends and New Low-Work-Function Boride and Nitride Materials for Electron Emission Applications. Journal of Physical Chemistry C, 2021, 125, 17400-17410.	3.1	13
10	Solid-phase epitaxial growth of the correlated-electron transparent conducting oxide $SrVO_3$. Physical Review Materials, 2021, 5, .	2.4	9
11	Graph network based deep learning of bandgaps. Journal of Chemical Physics, 2021, 155, 154702.	3.0	12
12	Modified band alignment method to obtain hybrid functional accuracy from standard DFT: Application to defects in highly mismatched III-V:Bi alloys. Physical Review Materials, 2021, 5, .	2.4	2
13	Understanding the interplay of surface structure and work function in oxides: A case study on SrTiO3. APL Materials, 2020, 8, .	5.1	20
14	Opportunities and Challenges for Machine Learning in Materials Science. Annual Review of Materials Research, 2020, 50, 71-103.	9.3	183
15	The Materials Simulation Toolkit for Machine learning (MAST-ML): An automated open source toolkit to accelerate data-driven materials research. Computational Materials Science, 2020, 176, 109544.	3.0	42
16	Semi-adsorption-controlled growth window for half-Heusler FeVSb epitaxial films. Physical Review Materials, 2020, 4, .	2.4	7
17	The incommensurately modulated structures of low-temperature labradorite feldspars: a single-crystal X-ray and neutron diffraction study. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 93-107.	1.1	4
18	Error assessment and optimal cross-validation approaches in machine learning applied to impurity diffusion. Computational Materials Science, 2019, 169, 109075.	3.0	42

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19	Massive Vacancy Concentration Yields Strong Room-Temperature Ferromagnetism in Two-Dimensional ZnO. Nano Letters, 2019, 19, 7085-7092.	9.1	31
20	Valleyite: A new magnetic mineral with the sodalite-type structure. American Mineralogist, 2019, 104, 1238-1245.	1.9	11
21	Exploring effective charge in electromigration using machine learning. MRS Communications, 2019, 9, 567-575.	1.8	18
22	Tuning perovskite oxides by strain: Electronic structure, properties, and functions in (electro)catalysis and ferroelectricity. Materials Today, 2019, 31, 100-118.	14.2	169
23	Materials Discovery of Stable and Nontoxic Halide Perovskite Materials for High‐Efficiency Solar Cells. Advanced Functional Materials, 2019, 29, 1804354.	14.9	61
24	New frontiers for the materials genome initiative. Npj Computational Materials, 2019, 5, .	8.7	312
25	Assessing Correlations of Perovskite Catalytic Performance with Electronic Structure Descriptors. Chemistry of Materials, 2019, 31, 785-797.	6.7	106
26	The incommensurately modulated structures of volcanic plagioclase: displacement, ordering and phase transition. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 643-656.	1.1	5
27	Frontiers in Thermionic Cathode Research. IEEE Transactions on Electron Devices, 2018, 65, 2061-2071.	3.0	70
28	Strain control of oxygen kinetics in the Ruddlesden-Popper oxide La1.85Sr0.15CuO4. Nature Communications, 2018, 9, 92.	12.8	38
29	Material Discovery and Design Principles for Stable, High Activity Perovskite Cathodes for Solid Oxide Fuel Cells. Advanced Energy Materials, 2018, 8, 1702708.	19.5	125
30	Predicting the thermodynamic stability of perovskite oxides using machine learning models. Computational Materials Science, 2018, 150, 454-463.	3.0	156
31	Factors Controlling Oxygen Interstitial Diffusion in the Ruddlesden‐Popper Oxide $La_{2-x}Sr_xNiO_{4+\delta}$. Chemistry of Materials, 2018, 30, 7166-7177.	6.7	28
32	Combining theory and experiment to model electron emission from polycrystalline tungsten cathode surfaces. , 2018, , .		2
33	Data and Supplemental information for predicting the thermodynamic stability of perovskite oxides using machine learning models. Data in Brief, 2018, 19, 261-263.	1.0	13
34	Combined ab initio and empirical model of the thermal conductivity of uranium, uranium-zirconium, and uranium-molybdenum. Physical Review Materials, 2018, 2, .	2.4	9
35	Stretching Epitaxial $La_{0.6}Sr_{0.4}CoO_{3-\delta}$ for Fast Oxygen Reduction. Journal of Physical Chemistry C, 2017, 121, 25651-25658.	3.1	38
36	Identification and Quantification of Boron Dopant Sites in Antiferromagnetic Cr2O3 Films by Electron Energy Loss Spectroscopy. Microscopy and Microanalysis, 2017, 23, 1584-1585.	0.4	2

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37	Work function and surface stability of tungsten-based thermionic electron emission cathodes. APL Materials, 2017, 5, .	5.1	52
38	High-throughput computational screening for low work function perovskite electron emitters. , 2017, , .		1
39	Understanding and Controlling the Work Function of Perovskite Oxides Using Density Functional Theory. Advanced Functional Materials, 2016, 26, 5471-5482.	14.9	127
40	Counterintuitive Reconstruction of the Polar O-Terminated ZnO Surface with Zinc Vacancies and Hydrogen. Journal of Physical Chemistry Letters, 2016, 7, 4483-4487.	4.6	19
41	Origins of Large Voltage Hysteresis in High-Energy-Density Metal Fluoride Lithium-Ion Battery Conversion Electrodes. Journal of the American Chemical Society, 2016, 138, 2838-2848.	13.7	212