Alexie M Kolpak

List of Publications by Year
in descending order

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33	3,822	257101 24	377514 34
papers	citations	h-index	g-index

35	35	35	5808
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Water electrolysis on La1â^'xSrxCoO3â^'Î´ perovskite electrocatalysts. Nature Communications, 2016, 7, 11053.	5.8	800
2	Remote epitaxy through graphene enables two-dimensional material-based layer transfer. Nature, 2017, 544, 340-343.	13.7	410
3	A Fundamental Relationship between Reaction Mechanism and Stability in Metal Oxide Catalysts for Oxygen Evolution. ACS Catalysis, 2016, 6, 1153-1158.	5.5	377
4	Role of Lattice Oxygen Participation in Understanding Trends in the Oxygen Evolution Reaction on Perovskites. ACS Catalysis, 2018, 8, 4628-4636.	5.5	339
5	Templated assembly of photoswitches significantly increases the energy-storage capacity of solar thermal fuels. Nature Chemistry, 2014, 6, 441-447.	6.6	261
6	Azobenzene-Functionalized Carbon Nanotubes As High-Energy Density Solar Thermal Fuels. Nano Letters, 2011, 11, 3156-3162.	4.5	228
7	On-the-fly active learning of interpretable Bayesian force fields for atomistic rare events. Npj Computational Materials, 2020, 6, .	3.5	199
8	Understanding the Composition and Activity of Electrocatalytic Nanoalloys in Aqueous Solvents: A Combination of DFT and Accurate Neural Network Potentials. Nano Letters, 2014, 14, 2670-2676.	4.5	180
9	Exceptional electrocatalytic oxygen evolution via tunable charge transfer interactions in La0.5Sr1.5Ni1â^'xFexO4Â±Î´ Ruddlesden-Popper oxides. Nature Communications, 2018, 9, 3150.	5.8	161
10	Discovering charge density functionals and structure-property relationships with PROPhet: A general framework for coupling machine learning and first-principles methods. Scientific Reports, 2017, 7, 1192.	1.6	98
11	Grand canonical molecular dynamics simulations of Cuâ€“Au nanoalloys in thermal equilibrium using reactive ANN potentials. Computational Materials Science, 2015, 110, 20-28.	1.4	93
12	Thickness-Dependent Photoelectrochemical Water Splitting on Ultrathin LaFeO₃ Films Grown on Nb:SrTiO₃. Journal of Physical Chemistry Letters, 2015, 6, 977-985.	2.1	75
13	Hybrid chromophore/template nanostructures: A customizable platform material for solar energy storage and conversion. Journal of Chemical Physics, 2013, 138, 034303.	1.2	71
14	Ab Initio Approach for Prediction of Oxide Surface Structure, Stoichiometry, and Electrocatalytic Activity in Aqueous Solution. Journal of Physical Chemistry Letters, 2015, 6, 1785-1789.	2.1	64
15	Electronic Origin and Kinetic Feasibility of the Lattice Oxygen Participation During the Oxygen Evolution Reaction on Perovskites. Journal of Physical Chemistry Letters, 2018, 9, 1473-1479.	2.1	62
16	Xâ€ray Transient Absorption and Picosecond IR Spectroscopy of Fulvalene(tetracarbonyl)diruthenium on Photoexcitation. Angewandte Chemie - International Edition, 2012, 51, 7692-7696.	7.2	47
17	Engineering Transitionâ€Metalâ€Coated Tungsten Carbides for Efficient and Selective Electrochemical Reduction of CO₂ to Methane. ChemSusChem, 2015, 8, 2745-2751.	3.6	43
18	Understanding photocatalytic overall water splitting on CoO nanoparticles: Effects of facets, surface stoichiometry, and the CoO/water interface. Journal of Catalysis, 2018, 365, 115-124.	3.1	39

#	Article	IF	Citations
19	Catalytic Activity and Product Selectivity Trends for Carbon Dioxide Electroreduction on Transition Metal-Coated Tungsten Carbides. Journal of Physical Chemistry C, 2017, 121, 20306-20314.	1.5	35
20	Reduced overpotentials for electrocatalytic water splitting over Fe- and Ni-modified BaTiO₃. Physical Chemistry Chemical Physics, 2016, 18, 29561-29570.	1.3	29
21	Mechanism for spontaneous oxygen and hydrogen evolution reactions on CoO nanoparticles. Journal of Materials Chemistry A, 2019, 7, 6708-6719.	5.2	29
22	Phonon Conduction in Silicon Nanobeam Labyrinths. Scientific Reports, 2017, 7, 6233.	1.6	28
23	Optimal methodology for explicit solvation prediction of band edges of transition metal oxide photocatalysts. Communications Chemistry, 2019, 2, .	2.0	28
24	Single Atomic Layer Ferroelectric on Silicon. Nano Letters, 2018, 18, 241-246.	4.5	26
25	Improved description of perovskite oxide crystal structure and electronic properties using self-consistent Hubbard <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math> corrections from ACBN0. Physical Review B, 2020, 101, .	1.1	17
26	Predicting HSE band gaps from PBE charge densities via neural network functionals. Journal of Physics Condensed Matter, 2020, 32, 155901.	0.7	16
27	Growth and interfacial properties of epitaxial oxides on semiconductors: ab initio insights. Journal of Materials Science, 2012, 47, 7417-7438.	1.7	12
28	PbTiO₃(001) Capped with ZnO(112Ì…0): An ab Initio Study of Effect of Substrate Polarization on Interface Composition and CO₂ Dissociation. Journal of Physical Chemistry Letters, 2016, 7, 1310-1314.	2.1	12
29	Thermal anisotropy enhanced by phonon size effects in nanoporous materials. Applied Physics Letters, 2017, 110, .	1.5	11
30	Photocatalytic hydrogen evolution activity of Co/CoO hybrid structures: a first-principles study on the Co layer thickness effect. Journal of Materials Chemistry A, 2019, 7, 16176-16189.	5.2	10
31	Directional Phonon Suppression Function as a Tool for the Identification of Ultralow Thermal Conductivity Materials. Scientific Reports, 2017, 7, 44379.	1.6	7
32	Control of valence and conduction band energies in layered transition metal phosphates via surface functionalization. Physical Chemistry Chemical Physics, 2016, 18, 14122-14128.	1.3	5
33	First-principles design of nanostructured hybrid photovoltaics based on layered transition metal phosphates. Scientific Reports, 2017, 7, 1248.	1.6	1