Alexie M Kolpak

List of Publications by Year
in descending order

33 papers	3,822 citations	257101 24 h-index	377514 34 g-index
35 all docs	35 docs citations	35 times ranked	5808 citing authors

#	Article	IF	Citations
1	Predicting HSE band gaps from PBE charge densities via neural network functionals. Journal of Physics Condensed Matter, 2020, 32, 155901.	0.7	16
2	On-the-fly active learning of interpretable Bayesian force fields for atomistic rare events. Npj Computational Materials, 2020, 6, .	3.5	199
3	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
4	Optimal methodology for explicit solvation prediction of band edges of transition metal oxide photocatalysts. Communications Chemistry, 2019, 2, .	2.0	28
5	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
6	Mechanism for spontaneous oxygen and hydrogen evolution reactions on CoO nanoparticles. Journal of Materials Chemistry A, 2019, 7, 6708-6719.	5.2	29
7	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
8	Role of Lattice Oxygen Participation in Understanding Trends in the Oxygen Evolution Reaction on Perovskites. ACS Catalysis, 2018, 8, 4628-4636.	5.5	339
9	Single Atomic Layer Ferroelectric on Silicon. Nano Letters, 2018, 18, 241-246.	4.5	26
10	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
11	Exceptional electrocatalytic oxygen evolution via tunable charge transfer interactions in La0.5Sr1.5Ni1âˆ'xFexO4Â±Î´ Ruddlesden-Popper oxides. Nature Communications, 2018, 9, 3150.	5.8	161
12	Remote epitaxy through graphene enables two-dimensional material-based layer transfer. Nature, 2017, 544, 340-343.	13.7	410
13	Directional Phonon Suppression Function as a Tool for the Identification of Ultralow Thermal Conductivity Materials. Scientific Reports, 2017, 7, 44379.	1.6	7
14	Thermal anisotropy enhanced by phonon size effects in nanoporous materials. Applied Physics Letters, 2017, 110, .	1.5	11
15	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
16	Phonon Conduction in Silicon Nanobeam Labyrinths. Scientific Reports, 2017, 7, 6233.	1.6	28
17	First-principles design of nanostructured hybrid photovoltaics based on layered transition metal phosphates. Scientific Reports, 2017, 7, 1248.	1.6	1
18	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

#	Article	IF	Citations
19	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
20	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
21	Reduced overpotentials for electrocatalytic water splitting over Fe- and Ni-modified BaTiO₃. Physical Chemistry Chemical Physics, 2016, 18, 29561-29570.	1.3	29
22	Water electrolysis on La1âˆ’xSrxCoO3âˆ’Î´ perovskite electrocatalysts. Nature Communications, 2016, 7, 11053.	5.8	800
23	A Fundamental Relationship between Reaction Mechanism and Stability in Metal Oxide Catalysts for Oxygen Evolution. ACS Catalysis, 2016, 6, 1153-1158.	5.5	377
24	Engineering Transitionâ€Metalâ€Coated Tungsten Carbides for Efficient and Selective Electrochemical Reduction of CO₂ to Methane. ChemSusChem, 2015, 8, 2745-2751.	3.6	43
25	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
26	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
27	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
28	Templated assembly of photoswitches significantly increases the energy-storage capacity of solar thermal fuels. Nature Chemistry, 2014, 6, 441-447.	6.6	261
29	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
30	Hybrid chromophore/template nanostructures: A customizable platform material for solar energy storage and conversion. Journal of Chemical Physics, 2013, 138, 034303.	1.2	71
31	Growth and interfacial properties of epitaxial oxides on semiconductors: ab initio insights. Journal of Materials Science, 2012, 47, 7417-7438.	1.7	12
32	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
33	Azobenzene-Functionalized Carbon Nanotubes As High-Energy Density Solar Thermal Fuels. Nano Letters, 2011, 11, 3156-3162.	4.5	228