Jeremy P Allen

List of Publications by Year
in descending order

18 papers	1,092 citations	567281 15 h-index	794594 19 g-index
19 all docs	19 docs citations	19 times ranked	2037 citing authors

#	Article	IF	Citations
1	Occupation matrix control of d- and f-electron localisations using DFT + U. Physical Chemistry Chemical Physics, 2014, 16, 21016-21031.	2.8	160
2	Origin of the Bipolar Doping Behavior of SnO from X-ray Spectroscopy and Density Functional Theory. Chemistry of Materials, 2013, 25, 3114-3123.	6.7	135
3	Geometry, Electronic Structure, and Bonding in CuMCh₂(M = Sb, Bi; Ch = S, Se): Alternative Solar Cell Absorber Materials?. Journal of Physical Chemistry C, 2012, 116, 7334-7340.	3.1	97
4	Tin Monoxide: Structural Prediction from First Principles Calculations with van der Waals Corrections. Journal of Physical Chemistry C, 2011, 115, 19916-19924.	3.1	95
5	The electronic structure of the antimony chalcogenide series: Prospects for optoelectronic applications. Journal of Solid State Chemistry, 2014, 213, 116-125.	2.9	86
6	Electronic Structures of Antimony Oxides. Journal of Physical Chemistry C, 2013, 117, 14759-14769.	3.1	80
7	Understanding the defect chemistry of tin monoxide. Journal of Materials Chemistry C, 2013, 1, 8194.	5.5	75
8	Electronic structure of mixed-valence silver oxide AgO from hybrid density-functional theory. Physical Review B, 2010, 81, .	3.2	71
9	Structure and Reducibility of CeO₂ Doped with Trivalent Cations. Journal of Physical Chemistry C, 2016, 120, 23430-23440.	3.1	66
10	Electronic structures of silver oxides. Physical Review B, 2011, 84, .	3.2	62
11	The Structure and Dynamics of Hydrated and Hydroxylated Magnesium Oxide Nanoparticles. Langmuir, 2011, 27, 1821-1829.	3.5	36
12	Atomistic Simulation of the Surface Carbonation of Calcium and Magnesium Oxide Surfaces. Journal of Physical Chemistry C, 2009, 113, 8320-8328.	3.1	30
13	Comparison of the defective pyrochlore and ilmenite polymorphs of AgSb<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>O</mml:mi><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow> GGA and hybrid DFT. Physical Review B, 2011, 83, .	3.2	23
14	Atomistic modelling of adsorption and segregation at inorganic solid interfaces. Molecular Simulation, 2009, 35, 584-608.	2.0	22
15	Atomistic Simulation of Surface Selectivity on Carbonate Formation at Calcium and Magnesium Oxide Surfaces. Journal of Physical Chemistry C, 2012, 116, 13240-13251.	3.1	21
16	Valence States in CeVO₄ and Ce_{0.5}Bi_{0.5}VO₄ Probed by Density Functional Theory Calculations and X-ray Photoemission Spectroscopy. Journal of Physical Chemistry C, 2014, 118, 25330-25339.	3.1	14
17	Electronic Structure of Epitaxial Sn-Doped Anatase Grown on SrTiO₃(001) by Dip Coating. Journal of Physical Chemistry C, 2013, 117, 15221-15228.	3.1	10
18	Layered CeSO and LiCeSO Oxide Chalcogenides Obtained via Topotactic Oxidative and Reductive Transformations. Inorganic Chemistry, 2019, 58, 3838-3850.	4.0	8