Anuj Goyal

List of Publications by Year in descending order

18 papers	908 citations	687363 13 h-index	839539 18 g-index
24 all docs	24 docs citations	24 times ranked	1647 citing authors

#	Article	IF	Citations
1	Formation of 6H-Ba₃Ce_{0.75}Mn_{2.25}O₉ during Thermochemical Reduction of 12R-Ba₄CeMn₃O₁₂: Identification of a Polytype in the Ba(Ce,Mn)O₃ Family. Inorganic Chemistry, 2022, 61, 6128-6137.	4.0	6
2	The influence of alloying on the stacking fault energy of gold from density functional theory calculations. Computational Materials Science, 2021, 188, 110236.	3.0	11
3	A data fusion approach to optimize compositional stability of halide perovskites. Matter, 2021, 4, 1305-1322.	10.0	75
4	Computational Fermi level engineering and doping-type conversion of Mg:Ga2O3 via three-step synthesis process. Journal of Applied Physics, 2021, 129, .	2.5	14
5	On the Dopability of Semiconductors and Governing Material Properties. Chemistry of Materials, 2020, 32, 4467-4480.	6.7	34
6	A simple chemical guide for finding novel n-type dopable Zintl pnictide thermoelectric materials. Journal of Materials Chemistry A, 2019, 7, 19385-19395.	10.3	29
7	Insights into operational stability and processing of halide perovskite active layers. Energy and Environmental Science, 2019, 12, 1341-1348.	30.8	125
8	The importance of phase equilibrium for doping efficiency: iodine doped PbTe. Materials Horizons, 2019, 6, 1444-1453.	12.2	42
9	The Conundrum of Relaxation Volumes in First-Principles Calculations of Charged Defects in UO2. Applied Sciences (Switzerland), 2019, 9, 5276.	2.5	11
10	Origin of Pronounced Nonlinear Band Gap Behavior in Leadâ€“Tin Hybrid Perovskite Alloys. Chemistry of Materials, 2018, 30, 3920-3928.	6.7	166
11	Metastable rocksalt ZnO is <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>p</mml:mi></mml:math> -type dopable. Physical Review Materials, 2018, 2, .	2.4	15
12	Capturing Anharmonicity in a Lattice Thermal Conductivity Model for High-Throughput Predictions. Chemistry of Materials, 2017, 29, 2494-2501.	6.7	88
13	A computational framework for automation of point defect calculations. Computational Materials Science, 2017, 130, 1-9.	3.0	131
14	First-principles calculation of intrinsic defect chemistry and self-doping in PbTe. Npj Computational Materials, 2017, 3, .	8.7	62
15	Nanoindentation of gold and gold alloys by molecular dynamics simulation. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2016, 651, 346-357.	5.6	54
16	Charge optimized many-body potential for aluminum. Journal of Physics Condensed Matter, 2015, 27, 015003.	1.8	7
17	Impact of homogeneous strain on uranium vacancy diffusion in uranium dioxide. Physical Review B, 2015, 91, .	3.2	27
18	Segregation of ruthenium to edge dislocations in uranium dioxide. Journal of Nuclear Materials, 2013, 441, 96-102.	2.7	8