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	Origin of Pronounced Nonlinear Band Gap Behavior in Leadâ€“Tin Hybrid Perovskite Alloys. Chemistry of Materials, 2018, 30, 3920-3928.	6.7	166
2	A computational framework for automation of point defect calculations. Computational Materials Science, 2017, 130, 1-9.	3.0	131
3	Insights into operational stability and processing of halide perovskite active layers. Energy and Environmental Science, 2019, 12, 1341-1348.	30.8	125
4	Capturing Anharmonicity in a Lattice Thermal Conductivity Model for High-Throughput Predictions. Chemistry of Materials, 2017, 29, 2494-2501.	6.7	88
5	A data fusion approach to optimize compositional stability of halide perovskites. Matter, 2021, 4, 1305-1322.	10.0	75
6	First-principles calculation of intrinsic defect chemistry and self-doping in PbTe. Npj Computational Materials, 2017, 3, .	8.7	62
7	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
8	The importance of phase equilibrium for doping efficiency: iodine doped PbTe. Materials Horizons, 2019, 6, 1444-1453.	12.2	42
9	On the Dopability of Semiconductors and Governing Material Properties. Chemistry of Materials, 2020, 32, 4467-4480.	6.7	34
10	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
11	Impact of homogeneous strain on uranium vacancy diffusion in uranium dioxide. Physical Review B, 2015, 91, .	3.2	27
12	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
13	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
14	The Conundrum of Relaxation Volumes in First-Principles Calculations of Charged Defects in UO2. Applied Sciences (Switzerland), 2019, 9, 5276.	2.5	11
15	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
16	Segregation of ruthenium to edge dislocations in uranium dioxide. Journal of Nuclear Materials, 2013, 441, 96-102.	2.7	8
17	Charge optimized many-body potential for aluminum. Journal of Physics Condensed Matter, 2015, 27, 015003.	1.8	7
18	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