

Niraj K Nepal

List of Publications by Year in descending order

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14
papers

244
citations

932766

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996533

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15
all docs

15
docs citations

15
times ranked

220
citing authors

#	ARTICLE	IF	CITATIONS
1	Interpretations of ground-state symmetry breaking and strong correlation in wavefunction and density functional theories. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	53
2	Stretched or noded orbital densities and self-interaction correction in density functional theory. Journal of Chemical Physics, 2019, 150, 174102.	1.2	46
3	First-principles study of mechanical and electronic properties of bent monolayer transition metal dichalcogenides. Physical Review Materials, 2019, 3, .	0.9	28
4	Opening band gaps of low-dimensional materials at the meta-GGA level of density functional approximations. Physical Review Materials, 2021, 5, .	0.9	18
5	Constraint-based wave vector and frequency dependent exchange-correlation kernel of the uniform electron gas. Physical Review B, 2020, 101, .	1.1	17
6	Tunable band gaps and optical absorption properties of bent MoS2 nanoribbons. Scientific Reports, 2022, 12, 3008.	1.6	14
7	Rocksalt or cesium chloride: Investigating the relative stability of the cesium halide structures with random phase approximation based methods. Physical Review B, 2018, 97, .	1.1	13
8	The Fermiâ€™s self-interaction correction for ionization energies of organic molecules. Journal of Chemical Physics, 2020, 153, 184303.	1.2	12
9	Formation energy puzzle in intermetallic alloys: Random phase approximation fails to predict accurate formation energies. Physical Review B, 2020, 102, .	1.1	12
10	Treating different bonding situations: Revisiting Au-Cu alloys using the random phase approximation. Physical Review B, 2019, 100, .	1.1	10
11	First-principles wave-vector- and frequency-dependent exchange-correlation kernel for jellium at all densities. Physical Review B, 2022, 105, .	1.1	7
12	Describing adsorption of benzene, thiophene, and xenon on coinage metals by using the Zarembkaâ€™Kohn theory-based model. Journal of Chemical Physics, 2021, 154, 124705.	1.2	4
13	Bending as a control knob for the electronic and optical properties of phosphorene nanoribbons. Physical Review Materials, 2022, 6, .	0.9	4
14	Understanding plasmon dispersion in nearly free electron metals: Relevance of exact constraints for exchange-correlation kernels within time-dependent density functional theory. Physical Review B, 2020, 101, .	1.1	3