Sriram Goverapet Srinivasan

List of Publications by Year
in descending order

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25	998	471509	580821
papers	citations	17 h-index	25 g-index

26	26	26	1480
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Development of a ReaxFF Potential for Carbon Condensed Phases and Its Application to the Thermal Fragmentation of a Large Fullerene. Journal of Physical Chemistry A, 2015, 119, 571-580.	2.5	243
2	Molecular-Dynamics-Based Study of the Collisions of Hyperthermal Atomic Oxygen with Graphene Using the ReaxFF Reactive Force Field. Journal of Physical Chemistry A, 2011, 115, 13269-13280.	2.5	95
3	Thermal properties of fluorinated graphene. Physical Review B, 2013, 87, .	3.2	91
4	Oxygen Interactions with Silica Surfaces: Coupled Cluster and Density Functional Investigation and the Development of a New ReaxFF Potential. Journal of Physical Chemistry C, 2013, 117, 258-269.	3.1	74
5	Graphene to fluorographene and fluorographane: a theoretical study. Nanotechnology, 2013, 24, 035706.	2.6	69
6	Bulk and surface DFT investigations of inorganic halide perovskites screened using machine learning and materials property databases. Physical Chemistry Chemical Physics, 2019, 21, 19423-19436.	2.8	59
7	Large Scale Computational Chemistry Modeling of the Oxidation of Highly Oriented Pyrolytic Graphite. Journal of Physical Chemistry A, 2013, 117, 2692-2703.	2.5	44
8	Ni on the CeO₂(110) and (100) surfaces: adsorption vs. substitution effects on the electronic and geometric structures and oxygen vacancies. Physical Chemistry Chemical Physics, 2016, 18, 11139-11149.	2.8	38
9	Lead-free, stable mixed halide double perovskites Cs2AgBiBr6 and Cs2AgBiBr6â^'xClx â€“ A detailed theoretical and experimental study. Chemical Physics, 2020, 529, 110547.	1.9	38
10	A comparative study of surface energies and water adsorption on Ce-bastnÃsite, La-bastnÃsite, and calcite via density functional theory and water adsorption calorimetry. Physical Chemistry Chemical Physics, 2017, 19, 7820-7832.	2.8	30
11	Determination of a Density Functional Tight Binding Model with an Extended Basis Set and Three-Body Repulsion for Carbon Under Extreme Pressures and Temperatures. Journal of Physical Chemistry C, 2013, 117, 7885-7894.	3.1	28
12	Crystal Structures, Surface Stability, and Water Adsorption Energies of La-BastnÃsite via Density Functional Theory and Experimental Studies. Journal of Physical Chemistry C, 2016, 120, 16767-16781.	3.1	28
13	Direction dependent etching of diamond surfaces by hyperthermal atomic oxygen: A ReaxFF based molecular dynamics study. Carbon, 2015, 82, 314-326.	10.3	27
14	Applied machine learning for predicting the lanthanide-ligand binding affinities. Scientific Reports, 2020, 10, 14322.	3.3	22
15	Thermodynamic, Spectroscopic, and Computational Studies of f-Element Complexation by N-Hydroxyethyl-diethylenetriamine-N,Nâ€²,Nâ€³,Nâ€³-tetraacetic Acid. Inorganic Chemistry, 2017, 56, 1722-1733.	4.0	19
16	A Density Functional Tight Binding Model with an Extended Basis Set and Three-Body Repulsion for Hydrogen under Extreme Thermodynamic Conditions. Journal of Physical Chemistry A, 2014, 118, 5520-5528.	2.5	18
17	Absolute Molecular Orientation of Isopropanol at Ceria (100) Surfaces: Insight into Catalytic Selectivity from the Interfacial Structure. Journal of Physical Chemistry C, 2017, 121, 14137-14146.	3.1	18
18	Understanding flotation processes at the atomic scale using density functional theory â€“ A case study on adsorption of 2-Mercaptobenzothiazole on chalcopyrite and pyrite surfaces. Applied Surface Science, 2022, 579, 152112.	6.1	11

#	Article	IF	Citations
19	Mineralâ€“Water Interface Structure of Xenotime (YPO4) {100}. Journal of Physical Chemistry C, 2018, 122, 20232-20243.	3.1	10
20	Hydration structure and water exchange kinetics at xenotimeâ€“water interfaces: implications for rare earth minerals separation. Physical Chemistry Chemical Physics, 2020, 22, 7719-7727.	2.8	10
21	Interfacial structure in the liquidâ€“liquid extraction of rare earth elements by phosphoric acid ligands: a molecular dynamics study. Physical Chemistry Chemical Physics, 2020, 22, 4177-4192.	2.8	9
22	Differential Stabilization of the Metalâ€“Ligand Complexes between Organic and Aqueous Phases Drives the Selectivity of Phosphoric Acid Ligands toward Heavier Rare Earth Elements. Industrial & Engineering Chemistry Research, 2018, 57, 17209-17217.	3.7	7
23	Surface segregation in the AgAuCuPdPt high entropy alloy: insights from molecular simulations. Molecular Systems Design and Engineering, 2022, 7, 878-888.	3.4	6
24	A Statistical Learning Framework for Accelerated Bandgap Prediction of Inorganic Compounds. Journal of Electronic Materials, 2020, 49, 752-762.	2.2	3
25	Materials Design in Digital Era: Challenges and Opportunities. Transactions of the Indian Institute of Metals, 2019, 72, 2199-2208.	1.5	1