

Shyam Vyas

List of Publications by Year in descending order

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Version: 2024-02-01

10
papers

675
citations

1163117

8
h-index

1372567

10
g-index

13
all docs

13
docs citations

13
times ranked

989
citing authors

#	ARTICLE	IF	CITATIONS
1	Prediction of Solubility Parameters and Miscibility of Pharmaceutical Compounds by Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2011, 115, 2014-2023.	2.6	248
2	BTBPs versus BTPHens: Some Reasons for Their Differences in Properties Concerning the Partitioning of Minor Actinides and the Advantages of BTPHens. <i>Inorganic Chemistry</i> , 2013, 52, 4993-5005.	4.0	137
3	Structure, stability and morphology of stoichiometric ceria crystallites. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1998, 94, 427-434.	1.7	109
4	NMR and Computational Studies of Chiral Discrimination by Amylose Tris(3,5-dimethylphenylcarbamate). <i>Journal of Physical Chemistry B</i> , 2007, 111, 1189-1198.	2.6	53
5	Evaluating Competing Intermolecular Interactions through Molecular Electrostatic Potentials and Hydrogen-Bond Propensities. <i>Crystal Growth and Design</i> , 2018, 18, 466-478.	3.0	36
6	Multiscale simulation of xenon diffusion and grain boundary segregation in UO ₂ . <i>Journal of Nuclear Materials</i> , 2015, 462, 15-25.	2.7	32
7	Cadmium and indium defects in ceria and their interaction with oxygen vacancies and small polarons. <i>Physical Review B</i> , 1995, 52, 13214-13222.	3.2	25
8	Metastable solid solutions of alumina in magnesia. <i>Journal of Physics and Chemistry of Solids</i> , 1997, 58, 1619-1624.	4.0	18
9	The Surface Structure of CaF ₂ ; A Comparison of Techniques. <i>Molecular Simulation</i> , 2001, 26, 307-321.	2.0	9
10	Imputation of sensory properties using deep learning. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 1125-1140.	2.9	7