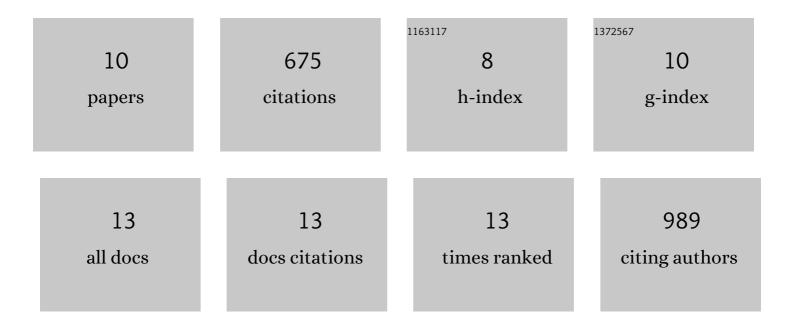
Shyam Vyas

List of Publications by Year in descending order

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SHAVA MAAAS

#	Article	IF	CITATIONS
1	Prediction of Solubility Parameters and Miscibility of Pharmaceutical Compounds by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 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. Inorganic Chemistry, 2013, 52, 4993-5005.	4.0	137
3	Structure, stability and morphology of stoichiometric ceria crystallites. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 427-434.	1.7	109
4	NMR and Computational Studies of Chiral Discrimination by Amylose Tris(3,5-dimethylphenylcarbamate). Journal of Physical Chemistry B, 2007, 111, 1189-1198.	2.6	53
5	Evaluating Competing Intermolecular Interactions through Molecular Electrostatic Potentials and Hydrogen-Bond Propensities. Crystal Growth and Design, 2018, 18, 466-478.	3.0	36
6	Multiscale simulation of xenon diffusion and grain boundary segregation in UO2. Journal of Nuclear Materials, 2015, 462, 15-25.	2.7	32
7	Cadmium and indium defects in ceria and their interaction with oxygen vacancies and small polarons. Physical Review B, 1995, 52, 13214-13222.	3.2	25
8	Metastable solid solutions of alumina in magnesia. Journal of Physics and Chemistry of Solids, 1997, 58, 1619-1624.	4.0	18
9	The Surface Structure of CaF2; A Comparison of Techniques. Molecular Simulation, 2001, 26, 307-321.	2.0	9
10	Imputation of sensory properties using deep learning. Journal of Computer-Aided Molecular Design, 2021, 35, 1125-1140.	2.9	7