

# Shyam Vyas

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/3512192/publications.pdf>

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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	Imputation of sensory properties using deep learning. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 1125-1140.	2.9	7
2	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
3	Multiscale simulation of xenon diffusion and grain boundary segregation in UO <sub>2</sub> . <i>Journal of Nuclear Materials</i> , 2015, 462, 15-25.	2.7	32
4	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
5	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
6	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
7	The Surface Structure of CaF <sub>2</sub> ; A Comparison of Techniques. <i>Molecular Simulation</i> , 2001, 26, 307-321.	2.0	9
8	Structure, stability and morphology of stoichiometric ceria crystallites. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1998, 94, 427-434.	1.7	109
9	Metastable solid solutions of alumina in magnesia. <i>Journal of Physics and Chemistry of Solids</i> , 1997, 58, 1619-1624.	4.0	18
10	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