

Xiya Lu

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

8

papers

487

citations

7

h-index

8

g-index

8

ext. papers

589

ext. citations

3.2

avg, IF

3.73

L-index

#	Paper	IF	Citations
8	Parameterization of DFTB3/3OB for Sulfur and Phosphorus for Chemical and Biological Applications. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 1518-1537	6.4	195
7	Parametrization of DFTB3/3OB for magnesium and zinc for chemical and biological applications. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 1062-82	3.4	90
6	Molecular simulation of water and hydration effects in different environments: challenges and developments for DFTB based models. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 11007-27	3.4	74
5	QM/MM free energy simulations: recent progress and challenges. <i>Molecular Simulation</i> , 2016 , 42, 1056-1078	6.3	63
4	Regulation and Plasticity of Catalysis in Enzymes: Insights from Analysis of Mechanochemical Coupling in Myosin. <i>Biochemistry</i> , 2017 , 56, 1482-1497	3.2	27
3	Charging free energy calculations using the Generalized Solvent Boundary Potential (GSBP) and periodic boundary condition: a comparative analysis using ion solvation and oxidation free energy in proteins. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 2005-18	3.4	26
2	Analysis of Phosphoryl-Transfer Enzymes with QM/MM Free Energy Simulations. <i>Methods in Enzymology</i> , 2018 , 607, 53-90	1.7	8
1	Analysis of Density Functional Tight Binding with Natural Bonding Orbitals. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 7439-7453	2.8	4