

Xiya Lu

List of Publications by Year in Descending Order

Source: <https://exaly.com/author-pdf/10684083/xiya-lu-publications-by-year.pdf>

Version: 2024-04-28

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

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	Analysis of Density Functional Tight Binding with Natural Bonding Orbitals. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 7439-7453	2.8	4
7	Analysis of Phosphoryl-Transfer Enzymes with QM/MM Free Energy Simulations. <i>Methods in Enzymology</i> , 2018 , 607, 53-90	1.7	8
6	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
5	QM/MM free energy simulations: recent progress and challenges. <i>Molecular Simulation</i> , 2016 , 42, 1056-1078		63
4	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
3	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
2	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
1	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