Zhiye Tang

List of Publications by Year
in descending order

13	296	1040056 9	1125743 13
papers	citations	h-index	g-index

20	20	20	426
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Potential Mean Force from Umbrella Sampling Simulations: What Can We Learn and What Is Missed?. Journal of Chemical Theory and Computation, 2019, 15, 2433-2443.	5.3	96
2	Binding Thermodynamics and Kinetics Calculations Using Chemical Host and Guest: A Comprehensive Picture of Molecular Recognition. Journal of Chemical Theory and Computation, 2018, 14, 303-318.	5.3	42
3	All-atom molecular dynamics study of impact fracture of glassy polymers. I: Molecular mechanism of brittleness of PMMA and ductility of PC. Polymer, 2019, 178, 121570.	3.8	34
4	All-atom molecular dynamics study of impact fracture of glassy polymers. II: Microscopic origins of stresses in elasticity, yielding, and strain hardening. Polymer, 2020, 207, 122908.	3.8	19
5	Transient States and Barriers from Molecular Simulations and the Milestoning Theory: Kinetics in Ligandâ€“Protein Recognition and Compound Design. Journal of Chemical Theory and Computation, 2020, 16, 1882-1895.	5.3	19
6	Adaptation of a Genetic Screen Reveals an Inhibitor for Mitochondrial Protein Import Component Tim44. Journal of Biological Chemistry, 2017, 292, 5429-5442.	3.4	18
7	Understanding ligand-receptor non-covalent binding kinetics using molecular modeling. Frontiers in Bioscience - Landmark, 2017, 22, 960-981.	3.0	18
8	Facet Selectivity of Ligands on Silver Nanoplates: Molecular Mechanics Study. Journal of Physical Chemistry C, 2014, 118, 21589-21598.	3.1	14
9	A molecular dynamics investigation of CDK8/CycC and ligand binding: conformational flexibility and implication in drug discovery. Journal of Computer-Aided Molecular Design, 2018, 32, 671-685.	2.9	12
10	Systematic Dissociation Pathway Searches Guided by Principal Component Modes. Journal of Chemical Theory and Computation, 2017, 13, 2230-2244.	5.3	7
11	An MM and QM Study of Biomimetic Catalysis of Diels-Alder Reactions Using Cyclodextrins. Catalysts, 2018, 8, 51.	3.5	5
12	A comparison of the brittle PMMA with the ductile PC on the elasticity and yielding from a molecular dynamics perspective. Polymer, 2021, 226, 123809.	3.8	5
13	All-atomistic molecular dynamics study of the glass transition of amorphous polymers. Polymer, 2022, 254, 125044.	3.8	2