Kento Kasahara

List of Publications by Year
in descending order

17	183	1307594 7	1125743 13
papers	citations	h-index	g-index

17	17	17	158
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Encounter complexes and hidden poses of kinase-inhibitor binding on the free-energy landscape. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 18404-18409.	7.1	41
2	New parallel computing algorithm of molecular dynamics for extremely huge scale biological systems. Journal of Computational Chemistry, 2021, 42, 231-241.	3.3	40
3	Reduced efficacy of a Src kinase inhibitor in crowded protein solution. Nature Communications, 2021, 12, 4099.	12.8	22
4	Optimized Hydrogen Mass Repartitioning Scheme Combined with Accurate Temperature/Pressure Evaluations for Thermodynamic and Kinetic Properties of Biological Systems. Journal of Chemical Theory and Computation, 2021, 17, 5312-5321.	5.3	15
5	Development of three-dimensional site-site Smoluchowski-Vlasov equation and application to electrolyte solutions. Journal of Chemical Physics, 2014, 140, 244110.	3.0	11
6	A theory of diffusion controlled reactions in polyatomic molecule system. Journal of Chemical Physics, 2016, 145, 194502.	3.0	9
7	Dynamics theory for molecular liquids based on an interaction site model. Physical Chemistry Chemical Physics, 2017, 19, 27917-27929.	2.8	9
8	A hybrid framework of first principles molecular orbital calculations and a three-dimensional integral equation theory for molecular liquids: Multi-center molecular Ornsteinâ€“Zernike self-consistent field approach. Journal of Chemical Physics, 2015, 143, 014103.	3.0	7
9	Solvent structure of ionic liquid with carbon dioxide. Journal of Molecular Liquids, 2016, 217, 12-16.	4.9	7
10	Theoretical Study of the Solvation Effect on the Reductive Reaction of Vinylene Carbonate in the Electrolyte Solution of Lithium Ion Batteries. Journal of Physical Chemistry B, 2017, 121, 5293-5299.	2.6	7
11	Solvation Structure of LiClO₄/Ethylene Carbonate Solution near a Graphite Electrode in Lithium-ion Batteries: 3D-RISM Study. Chemistry Letters, 2018, 47, 311-314.	1.3	4
12	Atomistic description of molecular binding processes based on returning probability theory. Journal of Chemical Physics, 2021, 155, 204503.	3.0	3
13	Timeâ€dependent pair distribution functions based on Smoluchowski equation and application to an electrolyte solution. Journal of Computational Chemistry, 2018, 39, 1491-1497.	3.3	2
14	Solvation in nitration of benzene and the valence electronic structure of the Wheland intermediate. Physical Chemistry Chemical Physics, 2022, 24, 16453-16461.	2.8	2
15	Crystal Growth of Urea and Its Modulation by Additives as Analyzed by All-Atom MD Simulation and Solution Theory. Journal of Physical Chemistry B, 2022, 126, 5274-5290.	2.6	2
16	A molecular level study of selective cation capture by a hostâ€“guest mechanism for 25,26,27,28-tetramethoxycalix[4]arene in MClO₄solution (MÂ=ÂNa, K). Molecular Simulation, 2015, 41, 881-891.	2.0	1
17	Constructing a Memory Kernel of the Returning Probability to Efficiently Describe Molecular Binding Processes. Chemistry Letters, 2022, 51, 823-827.	1.3	1