Niko Prasetyo

List of Publications by Year in descending order

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17	176	1163117 8	1125743 13
papers	citations	h-index	g-index

17	17	17	134
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantum Chemical and Monte Carlo Simulation Studies on Inhibition Performance of Caffeine and Its Derivatives against Corrosion of Copper. Coatings, 2020, 10, 1086.	2.6	34
2	Toward hydrogen storage material in fluorinated zirconium metal-organic framework (MOF-801): A periodic density functional theory (DFT) study of fluorination and adsorption. International Journal of Hydrogen Energy, 2021, 46, 4222-4228.	7.1	33
3	Lithium(I) in liquid ammonia: A quantum mechanical charge field (QMCF) molecular dynamics simulation study. Chemical Physics Letters, 2015, 619, 158-162.	2.6	19
4	Single-Ion Thermodynamics from First Principles: Calculation of the Absolute Hydration Free Energy and Single-Electrode Potential of Aqueous Li⁺ Using ab Initio Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2018, 14, 6443-6459.	5.3	18
5	Structure, Dynamics, and Hydration Free Energy of Carbon Dioxide in Aqueous Solution: A Quantum Mechanical/Molecular Mechanics Molecular Dynamics Thermodynamic Integration (QM/MM MD TI) Simulation Study. Journal of Chemical Theory and Computation, 2018, 14, 6472-6483.	5.3	15
6	Adsorption and dissociation of water molecules at the Î±-Al2O3(0001) surface: A 2-dimensional hybrid self-consistent charge density functional based tight-binding/molecular mechanics molecular dynamics (2D SCC-DFTB/MM MD) simulation study. Computational Materials Science, 2019, 164, 195-204.	3.0	12
7	Revisiting structure and dynamics of Ag+ in 18.6% aqueous ammonia: An ab initio quantum mechanical charge field simulation. Chemical Physics Letters, 2016, 652, 243-248.	2.6	11
8	Exploring structure and dynamics of solvated Ca(II) in liquid ammonia: A quantum mechanical charge field (QMCF) molecular dynamicsÂsimulation. Journal of Molecular Liquids, 2017, 242, 286-292.	4.9	11
9	Carbon dioxide in liquid ammonia: An ab initio Quantum Mechanical/Molecular Mechanical Molecular Dynamics Thermodynamic Integration (QM/MM MD TI) simulation study on structure, dynamics and thermodynamics of solvation. Journal of Molecular Liquids, 2020, 304, 112667.	4.9	6
10	Insight into the structure of the heulandite-type zeolite containing aromatic compounds using periodic density functional theory. Materials Today Communications, 2021, 26, 102028.	1.9	4
11	The effect of electron correlation in unraveling the hydration properties of Sc3+ in aqueous solution: A rigid body quantum mechanics/molecular mechanics simulation study. Journal of Molecular Liquids, 2021, 331, 115735.	4.9	4
12	Hybrid Forces Molecular Dynamics on the Lability, Dynamics and â€œStructure Breaking Effectâ€•of Cs+ in Liquid Ammonia. Bulletin of the Chemical Society of Japan, 2021, 94, 204-208.	3.2	3
13	Lability of the first solvation shell of silver cations in liquid ammonia: A quantum mechanical charge field molecular dynamics simulation study. Journal of Molecular Liquids, 2022, 350, 118517.	4.9	2
14	Irregular structure of the hydrated Ag+ in aqueous solution and its Dynamics: An insight from perturbation theory hybrid forces molecular dynamics simulation. Journal of Molecular Liquids, 2022, 361, 119688.	4.9	2
15	First solvation shell structure and dynamics of solvated Ca2+ in dilute aqueous ammonia by first principle approach: a QMCF MD simulation study. Monatshefte FÃ¼r Chemie, 2020, 151, 1493-1500.	1.8	1
16	Effect of Pt cluster size on CO2 adsorption and activation on (110) and (100) Î³-alumina surfaces: insights from DFT using a periodic boundary approach. Journal of Molecular Modeling, 2022, 28, 137.	1.8	1
17	Fate of Water Molecules on (11-20) and (1-102) Î±-Alumina Surfaces: 2D Periodic Self-Consistent Charge-Density Functional Tight-Binding/Molecular Mechanics Molecular Dynamics Study. Journal of Physical Chemistry C, 2022, 126, 11148-11157.	3.1	0