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	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
2	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
3	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
4	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
5	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
6	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
7	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
8	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
9	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
10	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
11	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
12	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
13	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
14	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
15	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
16	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
17	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