Eok Kyun Lee

List of Publications by Year
in descending order

20	388	840776 11	794594 19
papers	citations	h-index	g-index

21	21	21	737
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Tuned Chemical Bonding Ability of Au at Grain Boundaries for Enhanced Electrochemical CO₂ Reduction. ACS Catalysis, 2016, 6, 4443-4448.	11.2	103
2	Brownian motion from molecular dynamics. Chemical Physics, 2010, 375, 316-326.	1.9	69
3	Nature of intrinsic uncertainties in equilibrium molecular dynamics estimation of shear viscosity for simple and complex fluids. Journal of Chemical Physics, 2018, 149, 044510.	3.0	30
4	uMBD: A Materials-Ready Dispersion Correction That Uniformly Treats Metallic, Ionic, and van der Waals Bonding. Journal of the American Chemical Society, 2020, 142, 2346-2354.	13.7	29
5	First-Principles Study of the Î±â€“Î² Phase Transition of Ferroelectric Poly(vinylidene difluoride): Observation of Multiple Transition Pathways. Journal of Physical Chemistry B, 2016, 120, 3240-3249.	2.6	21
6	Recent development of atomâ€pairwise van der waals corrections for density functional theory: From molecules to solids. International Journal of Quantum Chemistry, 2016, 116, 598-607.	2.0	19
7	Layer-wise relevance propagation of InteractionNet explains proteinâ€“ligand interactions at the atom level. Scientific Reports, 2020, 10, 21155.	3.3	15
8	Qubit Geometry and Conformal Mapping. Quantum Information Processing, 2002, 1, 129-134.	2.2	12
9	Normal versus anomalous self-diffusion in two-dimensional fluids: Memory function approach and generalized asymptotic Einstein relation. Journal of Chemical Physics, 2014, 141, 214112.	3.0	12
10	Electronic Structure and Band Alignments of Various Phases of Titania Using the Self-Consistent Hybrid Density Functional and DFT+U Methods. Frontiers in Chemistry, 2019, 7, 47.	3.6	12
11	Theoretical study of the microscopic origin of magnetocrystalline anisotropy in Fe₁₆N₂ and its alloys: comparison with the other L1₀ alloys. Journal of Physics Condensed Matter, 2020, 32, 035801.	1.8	12
12	Density-dependent finite system-size effects in equilibrium molecular dynamics estimation of shear viscosity: Hydrodynamic and configurational study. Journal of Chemical Physics, 2019, 151, 104101.	3.0	10
13	Molecular hydrodynamics: Vortex formation and sound wave propagation. Journal of Chemical Physics, 2018, 148, 024506.	3.0	9
14	DYNAMICS OF SIMPLE FLUIDS CONFINED IN CYLINDRICAL PORE: EFFECT OF PORE SIZE. Journal of Theoretical and Computational Chemistry, 2005, 04, 305-315.	1.8	7
15	Nature of self-diffusion in two-dimensional fluids. New Journal of Physics, 2017, 19, 123038.	2.9	7
16	First-Principles Studies on Twinnability of Magnesium Alloys: Effects of Yttrium and Lithium on $$left({10ar{1}1} ight)left[{ar{1}012} ight]$$ 10 1. Metals and Materials International, 2018, 24, 720-729.	3.4	6
17	Rotational Varianceâ€Based Data Augmentation in 3D Graph Convolutional Network. Chemistry - an Asian Journal, 2021, 16, 2610-2613.	3.3	6
18	Density functional study of Î±â€“Î² phase transition of polyvinylidene difluoride. Physica Status Solidi - Rapid Research Letters, 2012, 6, 217-219.	2.4	4

#	Article	IF	Citations
19	Effects of Pooling Operations on Prediction of Ligand Rotationâ€Dependent Proteinâ€“Ligand Binding in 3D Graph Convolutional Network. Bulletin of the Korean Chemical Society, 2021, 42, 744-747.	1.9	4
20	Negative tunneling magnetoresistance in spin filtering magnetic junctions with spin-orbit coupling. , 2010, , .		1