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	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
2	Rotational Varianceâ€Based Data Augmentation in 3D Graph Convolutional Network. Chemistry - an Asian Journal, 2021, 16, 2610-2613.	3.3	6
3	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
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	Layer-wise relevance propagation of InteractionNet explains proteinâ€“ligand interactions at the atom level. Scientific Reports, 2020, 10, 21155.	3.3	15
6	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
7	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
8	Molecular hydrodynamics: Vortex formation and sound wave propagation. Journal of Chemical Physics, 2018, 148, 024506.	3.0	9
9	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
10	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
11	Nature of self-diffusion in two-dimensional fluids. New Journal of Physics, 2017, 19, 123038.	2.9	7
12	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
13	Tuned Chemical Bonding Ability of Au at Grain Boundaries for Enhanced Electrochemical CO₂ Reduction. ACS Catalysis, 2016, 6, 4443-4448.	11.2	103
14	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
15	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
16	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
17	Brownian motion from molecular dynamics. Chemical Physics, 2010, 375, 316-326.	1.9	69
18	Negative tunneling magnetoresistance in spin filtering magnetic junctions with spin-orbit coupling. , 2010, , .		1

#	Article	IF	Citations
19	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
20	Qubit Geometry and Conformal Mapping. Quantum Information Processing, 2002, 1, 129-134.	2.2	12