Won June Kim

List of Publications by Year
in descending order

20	421	759233 12	752698 20
papers	citations	h-index	g-index

21	21	21	694
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	Electro-synthesis of Ammonia from Dilute Nitric Oxide on a Gas Diffusion Electrode. ACS Energy Letters, 2022, 7, 958-965.	17.4	52
3	Adsorption mechanisms of fatty acids on fluorite unraveled by infrared spectroscopy and first-principles calculations. Journal of Colloid and Interface Science, 2021, 583, 692-703.	9.4	50
4	Benchmarking several van der Waals dispersion approaches for the description of intermolecular interactions. Journal of Chemical Physics, 2018, 148, 064112.	3.0	37
5	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
6	Benchmarking the performance of approximate van der Waals methods for the structural and energetic properties of SiO2 and AlPO4 frameworks. Journal of Chemical Physics, 2019, 150, 094102.	3.0	24
7	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
8	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
9	Cluster Expansion Method for Simulating Realistic Size of Nanoparticle Catalysts with an Application in CO₂ Electroreduction. Journal of Physical Chemistry C, 2018, 122, 9245-9254.	3.1	17
10	Failure of Density Functional Dispersion Correction in Metallic Systems and Its Possible Solution Using a Modified Many-Body Dispersion Correction. Journal of Physical Chemistry Letters, 2016, 7, 3278-3283.	4.6	13
11	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
12	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
13	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
14	Rotational Varianceâ€Based Data Augmentation in 3D Graph Convolutional Network. Chemistry - an Asian Journal, 2021, 16, 2610-2613.	3.3	6
15	Lifshitz Transition and Nonâ€Fermi Liquid Behavior in Highly Doped Semimetals. Advanced Materials, 2021, 33, 2005742.	21.0	5
16	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
17	First principles investigations of the optical selectivity of titanium carbide-based materials for concentrating solar power applications. Journal of Materials Chemistry C, 2021, 9, 7591-7598.	5.5	4
18	Electronic Structure of Heavy Halogen Atoms Adsorbed on the Cu(111) Surface: A Combined ARPES and First Principles Calculations Study. Journal of Physical Chemistry C, 2019, 123, 26309-26314.	3.1	3

#	Article	IF	Citations
19	MolNet: A Chemically Intuitive Graph Neural Network for Prediction of Molecular Properties. Chemistry - an Asian Journal, 2022, 17, .	3.3	3
20	Assessment and prediction of band edge locations of nitrides using a self-consistent hybrid functional. Journal of Chemical Physics, 2021, 155, 024120.	3.0	1