Kyuho Lee

List of Publications by Year in descending order

46 papers	7,654 citations	117625 34 h-index	223800 46 g-index
46 all docs	46 docs citations	46 times ranked	10380 citing authors

#	Article	IF	Citations
1	Performance of van der Waals Corrected Functionals for Guest Adsorption in the M₂(dobdc) Metalâ€“Organic Frameworks. Journal of Physical Chemistry A, 2017, 121, 4139-4151.	2.5	41
2	First-principles Hubbard U approach for small molecule binding in metal-organic frameworks. Journal of Chemical Physics, 2016, 144, 174104.	3.0	73
3	Force Field Development from Periodic Density Functional Theory Calculations for Gas Separation Applications Using Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2016, 120, 12590-12604.	3.1	95
4	Structural and excited-state properties of oligoacene crystals from first principles. Physical Review B, 2016, 93, .	3.2	89
5	Small-Molecule Adsorption in Open-Site Metalâ€“Organic Frameworks: A Systematic Density Functional Theory Study for Rational Design. Chemistry of Materials, 2015, 27, 668-678.	6.7	248
6	Cooperative insertion of CO2 in diamine-appended metal-organic frameworks. Nature, 2015, 519, 303-308.	27.8	1,026
7	CO₂ induced phase transitions in diamine-appended metalâ€“organic frameworks. Chemical Science, 2015, 6, 5177-5185.	7.4	45
8	van der Waals forces in density functional theory: a review of the vdW-DF method. Reports on Progress in Physics, 2015, 78, 066501.	20.1	615
9	van der Waals density functionals built upon the electron-gas tradition: Facing the challenge of competing interactions. Journal of Chemical Physics, 2014, 140, 18A539.	3.0	100
10	Oxidation of ethane to ethanol by N2O in a metalâ€“organic framework with coordinatively unsaturated iron(II) sites. Nature Chemistry, 2014, 6, 590-595.	13.6	398
11	Design of a Metalâ€“Organic Framework with Enhanced Back Bonding for Separation of N₂ and CH₄. Journal of the American Chemical Society, 2014, 136, 698-704.	13.7	157
12	Efficient Determination of Accurate Force Fields for Porous Materials Using ab Initio Total Energy Calculations. Journal of Physical Chemistry C, 2014, 118, 2693-2701.	3.1	23
13	Comprehensive study of carbon dioxide adsorption in the metalâ€“organic frameworks M₂(dobdc) (M = Mg, Mn, Fe, Co, Ni, Cu, Zn). Chemical Science, 2014, 5, 4569-4581.	7.4	342
14	CO₂ Adsorption in Fe₂(dobdc): A Classical Force Field Parameterized from Quantum Mechanical Calculations. Journal of Physical Chemistry C, 2014, 118, 12230-12240.	3.1	45
15	Force-Field Development from Electronic Structure Calculations with Periodic Boundary Conditions: Applications to Gaseous Adsorption and Transport in Metalâ€“Organic Frameworks. Journal of Chemical Theory and Computation, 2014, 10, 1477-1488.	5.3	121
16	Reversible CO Binding Enables Tunable CO/H₂ and CO/N₂ Separations in Metalâ€“Organic Frameworks with Exposed Divalent Metal Cations. Journal of the American Chemical Society, 2014, 136, 10752-10761.	13.7	210
17	Understanding Trends in CO₂ Adsorption in Metalâ€“Organic Frameworks with Open-Metal Sites. Journal of Physical Chemistry Letters, 2014, 5, 861-865.	4.6	139
18	Methane storage capabilities of diamond analogues. Physical Chemistry Chemical Physics, 2013, 15, 20937.	2.8	10

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19	Phase diagram of graphene nanoribbons and band-gap bifurcation of Dirac fermions under quantum confinement. Physical Review B, 2012, 85, .	3.2	16
20	Structure and energetics of a ferroelectric organic crystal of phenazine and chloranilic acid. Physical Review B, 2012, 86, .	3.2	24
21	First-principles theoretical study of organic/metal interfaces: Vacuum level shifts and interface dipoles. Current Applied Physics, 2012, 12, S2-S9.	2.4	18
22	Benchmarking van der Waals density functionals with experimental data: potential-energy curves for H₂molecules on Cu(111), (100) and (110) surfaces. Journal of Physics Condensed Matter, 2012, 24, 424213.	1.8	35
23	Altering the spin state of transition metal centers in metalâ€“organic frameworks by molecular hydrogen adsorption: a first-principles study. Physical Chemistry Chemical Physics, 2011, 13, 5042.	2.8	10
24	Density Functional Theoretical Study of Perfluoropentacene/Noble Metal Interfaces with van der Waals Corrections: Adsorption States and Vacuum Level Shifts. Journal of Physical Chemistry C, 2011, 115, 5767-5772.	3.1	23
25	Evaluation of a density functional with account of van der Waals forces using experimental data of H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>physisorption on Cu(111). Physical Review B, 2011, 84, .	3.2	46
26	Adsorption of Alq<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>on Mg(001) surface: Role of chemical bonding, molecular distortion, and van der Waals interaction. Physical Review B, 2011, 83, .	3.2	7
27	Higher-accuracy van der Waals density functional. Physical Review B, 2010, 82, .	3.2	2,072
28	Hole-Mediated Hydrogen Spillover Mechanism in Metal-Organic Frameworks. Physical Review Letters, 2010, 104, 236101.	7.8	34
29	Interaction of water with a metal surface: Importance of van der Waals forces. Physical Review B, 2010, 81, .	3.2	61
30	Accuracy of density functional theory methods for weakly bonded systems: The case of dihydrogen binding on metal centers. Physical Review B, 2010, 82, .	3.2	38
31	Stability of graphene oxide phases from first-principles calculations. Physical Review B, 2010, 82, .	3.2	124
32	Mapping Atomic Contact between Pentacene and a Au Surface using Scanning Tunneling Spectroscopy. Nano Letters, 2010, 10, 996-999.	9.1	13
33	Density functional theoretical study of pentacene/noble metal interfaces with van der Waals corrections: Vacuum level shifts and electronic structures. Journal of Chemical Physics, 2010, 132, 134703.	3.0	118
34	Adsorption of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>-butane on Cu(100), Cu(111), Au(111), and Pt(111): Van der Waals density-functional study. Physical Review B, 2010, 82, .	3.2	50
35	First-principles study of the pentacene/Cu(111) interface: Adsorption states and vacuum level shifts. Journal of Electron Spectroscopy and Related Phenomena, 2009, 174, 78-84.	1.7	45
36	First-principles study of benzene on noble metal surfaces: Adsorption states and vacuum level shifts. Surface Science, 2009, 603, 2912-2922.	1.9	82

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37	Graphene Oxide as an Ideal Substrate for Hydrogen Storage. ACS Nano, 2009, 3, 2995-3000.	14.6	342
38	Ab initio design of Ca-decorated organic frameworks for high capacity molecular hydrogen storage with enhanced binding. Applied Physics Letters, 2009, 95, 033109.	3.3	49
39	Investigation of Exchange Energy Density Functional Accuracy for Interacting Molecules. Journal of Chemical Theory and Computation, 2009, 5, 2754-2762.	5.3	282
40	Accurate and efficient calculation of van der Waals interactions within density functional theory by local atomic potential approach. Journal of Chemical Physics, 2008, 129, 154102.	3.0	73
41	First-principles theoretical study of Alq3âˆ•Al interfaces: Origin of the interfacial dipole. Journal of Chemical Physics, 2008, 128, 244704.	3.0	51
42	Comparison of localized basis and plane-wave basis for density-functional calculations of organic molecules on metals. Physical Review B, 2007, 75, .	3.2	64
43	Ab initio study of pentacene on Au(001) surface. Surface Science, 2005, 589, 8-18.	1.9	54
44	Band gap sensitivity of bromine adsorption at carbon nanotubes. Chemical Physics Letters, 2005, 403, 135-139.	2.6	30
45	Formation, Manipulation, and Elasticity Measurement of a Nanometric Column of Water Molecules. Physical Review Letters, 2005, 95, 187801.	7.8	84
46	Energetics of large carbon clusters:â€,â€,Crossover from fullerenes to nanotubes. Physical Review B, 2002, 65, .	3.2	32