Hoonkyung Lee

List of Publications by Year
in descending order

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91 papers	4,660 citations	136885 32 h-index	98753 67 g-index
93 all docs	93 docs citations	93 times ranked	5880 citing authors

#	Article	IF	Citations
1	Molecular beam epitaxial growth of Sb₂Te₃â€“Bi₂Te₃ lateral heterostructures. 2D Materials, 2022, 9, 025006.	2.0	6
2	Boronâ€Rich Boron Nitride Nanotubes as Highly Selective Adsorbents for Selected Diatomic Air Pollutants: A DFT Study. Advanced Theory and Simulations, 2022, 5, .	1.3	8
3	Ultrasensitive N-Channel Graphene Gas Sensors by Nondestructive Molecular Doping. ACS Nano, 2022, 16, 2176-2187.	7.3	42
4	High-capacity reversible hydrogen storage properties of metal-decorated nitrogenated holey graphenes. International Journal of Hydrogen Energy, 2022, 47, 10654-10664.	3.8	22
5	Two-Dimensional Bismuthene Nanosheets for Selective Detection of Toxic Gases. ACS Applied Nano Materials, 2022, 5, 2984-2993.	2.4	29
6	Highly Efficient Invisible TaO_x/ZTO Bilayer Memristor for Neuromorphic Computing and Image Sensing. ACS Applied Electronic Materials, 2022, 4, 2180-2190.	2.0	20
7	Selective decoration of nitrogenated holey graphene (C2N) with titanium clusters for enhanced hydrogen storage application. International Journal of Hydrogen Energy, 2021, 46, 7371-7380.	3.8	63
8	Density Functional Theory Study of Li-Functionalized Nanoporous R-Graphyneâ€“Metalâ€“Organic Frameworks for Reversible Hydrogen Storage. ACS Applied Nano Materials, 2021, 4, 3949-3957.	2.4	16
9	Two-dimensional Janus monolayers of MoSSe as promising sensor towards selected adulterants compounds. Applied Surface Science, 2021, 542, 148590.	3.1	29
10	Density Functional Theory Study on Sensing and Dielectric Properties of Arsenic Trisulfide Nanosheets for Detecting Volatile Organic Compounds. ACS Applied Nano Materials, 2021, 4, 5444-5453.	2.4	9
11	Unidirectional Alignment of AgCN Microwires on Distorted Transition Metal Dichalcogenide Crystals. ACS Applied Materials & Interfaces, 2021, 13, 8727-8735.	4.0	3
12	Wafer-Scale Production of Transition Metal Dichalcogenides and Alloy Monolayers by Nanocrystal Conversion for Large-Scale Ultrathin Flexible Electronics. Nano Letters, 2021, 21, 9153-9163.	4.5	29
13	Band gap engineering of 2D biphenylene carbon sheets with hydrogenation. Journal of the Korean Physical Society, 2021, 79, 846-850.	0.3	11
14	Conversion of CO₂ into Formic Acid on Transition Metal-Porphyrin-like Graphene: First Principles Calculations. ACS Omega, 2021, 6, 27045-27051.	1.6	3
15	Tunning Hydrogen Storage Properties of Carbon Eneâ€“Yne Nanosheets through Selected Foreign Metal Functionalization. Journal of Physical Chemistry C, 2020, 124, 16827-16837.	1.5	15
16	Selfâ€Powered Gas Sensors: 2D Transition Metal Dichalcogenide Heterostructures for pâ€•and nâ€Type Photovoltaic Selfâ€Powered Gas Sensor (Adv. Funct. Mater. 43/2020). Advanced Functional Materials, 2020, 30, 2070284.	7.8	1
17	2D Transition Metal Dichalcogenide Heterostructures for pâ€•and nâ€Type Photovoltaic Selfâ€Powered Gas Sensor. Advanced Functional Materials, 2020, 30, 2003360.	7.8	102
18	Efficient Sensing Properties of Aluminum Nitride Nanosheets toward Toxic Pollutants under Gated Electric Field. ACS Applied Electronic Materials, 2020, 2, 1645-1652.	2.0	15

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19	Doping effect in graphene-graphene oxide interlayer. Scientific Reports, 2020, 10, 8258.	1.6	25
20	Sensing of volatile organic compounds on two-dimensional nitrogenated holey graphene, graphdiyne, and their heterostructure. Carbon, 2020, 163, 213-223.	5.4	77
21	Critical differences in 3D atomic structure of individual ligand-protected nanocrystals in solution. Science, 2020, 368, 60-67.	6.0	103
22	Physisorption and Chemisorption of SF6 by Transition Metal-Porphyrin Structure Embedded on Graphene Surface with Different Hapticities. Journal of the Korean Physical Society, 2020, 76, 1001-1004.	0.3	1
23	Capacity enhancement of polylithiated functionalized boron nitride nanotubes: an efficient hydrogen storage medium. Physical Chemistry Chemical Physics, 2020, 22, 15675-15682.	1.3	18
24	Highly sensitive and selective sensing properties of modified green phosphorene monolayers towards SF6 decomposition gases. Applied Surface Science, 2020, 512, 145641.	3.1	28
25	Hydrogen storage capacity of low-lying isomer of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mrow><mml:msub><mml:mrow><mml:mtext>C</mml:mtext></mml:mrow><mml:mrow><mml:mn>24</mml:mn> functionalized with Ti. International Journal of Hydrogen Energy, 2020, 45, 9936-9945.	3.8	50
26	Universal Oriented van der Waals Epitaxy of 1D Cyanide Chains on Hexagonal 2D Crystals. Advanced Science, 2020, 7, 1900757.	5.6	13
27	Graphene-Based Ultrasensitive Strain Sensors. ACS Applied Electronic Materials, 2020, 2, 523-528.	2.0	11
28	Competition between HÃ¼ckelâ€™s Rule and Jahnâ€“Teller Distortion in Small Carbon Rings: A Quantum Monte Carlo Study. Journal of Physical Chemistry A, 2020, 124, 3636-3640.	1.1	13
29	Dielectric Constant and van der Waals Interlayer Interaction of MoS2-Graphene Heterostructures. , 2020, , .		5
30	Sensitivity enhancement of stanene towards toxic SO2 and H2S. Applied Surface Science, 2019, 495, 143622.	3.1	17
31	Textile-based high-performance hydrogen evolution of low-temperature atomic layer deposition of cobalt sulfide. Nanoscale, 2019, 11, 844-850.	2.8	17
32	Reversible hydrogen storage properties of defect-engineered <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="bold">C</mml:mi></mml:mrow><mml:mrow><mml:mn mathvariant="bold">4</mml:mn></mml:mrow></mml:msub><mml:mi mathvariant="bold">N</mml:mi></mml:mrow></mml:math> nanosheets under ambient conditions. Car	5.4	69
33	Enhancement in hydrogen storage capacities of light metal functionalized Boronâ€“Graphdiyne nanosheets. Carbon, 2019, 147, 199-205.	5.4	100
34	Molecular-Level Understanding of Continuous Growth from Iron-Oxo Clusters to Iron Oxide Nanoparticles. Journal of the American Chemical Society, 2019, 141, 7037-7045.	6.6	58
35	Pressure-induced phase transitions and superconductivity in magnesium carbides. Scientific Reports, 2019, 9, 20253.	1.6	4
36	Theoretical investigation of the vertical dielectric screening dependence on defects for few-layered van der Waals materials. RSC Advances, 2019, 9, 40309-40315.	1.7	12

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37	Raman Spectra Shift of Few-Layer IV-VI 2D Materials. Scientific Reports, 2019, 9, 19826.	1.6	36
38	Amorphous-Phase-Mediated Crystallization of Ni Nanocrystals Revealed by High-Resolution Liquid-Phase Electron Microscopy. Journal of the American Chemical Society, 2019, 141, 763-768.	6.6	76
39	Off-Plane Dielectric Screening of Few-Layer Graphdiyne and Its Family. ACS Applied Materials & Interfaces, 2019, 11, 2571-2578.	4.0	13
40	Enhanced Hydrogen-Storage Capacity and Structural Stability of an Organic Clathrate Structure with Fullerene (C₆₀) Guests and Lithium Doping. Chemistry of Materials, 2018, 30, 3028-3039.	3.2	22
41	Feâ€“Porphyrin-like Nanostructures for Selective Ammonia Capture under Humid Conditions. Journal of Physical Chemistry C, 2018, 122, 2046-2052.	1.5	7
42	Design of 2D massless Dirac fermion systems and quantum spin Hall insulators based on spâ€“sp2 carbon sheets. Npj Computational Materials, 2018, 4, .	3.5	20
43	One-Dimensional Assembly on Two-Dimensions: AuCN Nanowire Epitaxy on Graphene for Hybrid Phototransistors. Nano Letters, 2018, 18, 6214-6221.	4.5	30
44	spâ€“sp² Carbon Sheets as Promising Anode Materials for Na-Ion Batteries. ACS Omega, 2018, 3, 14477-14481.	1.6	6
45	Control of CO₂ Capture Process on Transition-Metal-Porphyrin-like Graphene with Mechanical Strain. ACS Omega, 2018, 3, 10554-10563.	1.6	7
46	Nature of Interlayer Binding and Stacking of spâ€“sp² Hybridized Carbon Layers: A Quantum Monte Carlo Study. Journal of Chemical Theory and Computation, 2017, 13, 5639-5646.	2.3	27
47	Vertical dielectric screening of few-layer van der Waals semiconductors. Nanoscale, 2017, 9, 14540-14547.	2.8	20
48	Calcium-decorated carbon nanostructures for the selective capture of carbon dioxide. Physical Chemistry Chemical Physics, 2016, 18, 29086-29091.	1.3	15
49	Improvement of Gas-Sensing Performance of Large-Area Tungsten Disulfide Nanosheets by Surface Functionalization. ACS Nano, 2016, 10, 9287-9296.	7.3	351
50	Steric effects of CO 2 binding to transition metal-benzene complexes: AÂfirst-principles study. Current Applied Physics, 2016, 16, 1124-1129.	1.1	8
51	High-throughput screening of metal-porphyrin-like graphenes for selective capture of carbon dioxide. Scientific Reports, 2016, 6, 21788.	1.6	31
52	Wedge energy bands of monolayer black phosphorus: a first-principles study. Journal of Physics Condensed Matter, 2016, 28, 305301.	0.7	1
53	Synthesis and mechanistic study of in situ halogen/nitrogen dual-doping in graphene tailored by stepwise pyrolysis of ionic liquids. Nanotechnology, 2015, 26, 115601.	1.3	7
54	Recent progress on Kubas-type hydrogen-storage nanomaterials: from theories to experiments. Journal of the Korean Physical Society, 2015, 66, 1649-1655.	0.3	25

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55	Graphene-templated directional growth of an inorganic nanowire. Nature Nanotechnology, 2015, 10, 423-428.	15.6	75
56	Configuration of ripple domains and their topological defects formed under local mechanical stress on hexagonal monolayer graphene. Scientific Reports, 2015, 5, 9390.	1.6	10
57	Exceptional Optoelectronic Properties of Hydrogenated Bilayer Silicene. Physical Review X, 2014, 4, .	2.8	35
58	DFT and TB study of the geometry of hydrogen adsorbed on graphynes. Journal of Physics Condensed Matter, 2014, 26, 385301.	0.7	2
59	Cohesion energetics of carbon allotropes: Quantum Monte Carlo study. Journal of Chemical Physics, 2014, 140, 114702.	1.2	166
60	Tailoring the Electronic Band Gap of Graphyne. Journal of Physical Chemistry C, 2014, 118, 2463-2468.	1.5	34
61	Widely tunable band gaps of graphdiyne: an ab initio study. Physical Chemistry Chemical Physics, 2014, 16, 8935-8939.	1.3	56
62	Origin of Poor Cyclability in Li₂MnSiO₄ from First-Principles Calculations: Layer Exfoliation and Unstable Cycled Structure. Chemistry of Materials, 2014, 26, 3896-3899.	3.2	45
63	Semiclassical approximation solved by Monte Carlo integration as an efficient impurity solver for dynamical mean field theory and its cluster extensions. Physical Review B, 2013, 88, .	1.1	4
64	Carbyne from First Principles: Chain of C Atoms, a Nanorod or a Nanorope. ACS Nano, 2013, 7, 10075-10082.	7.3	375
65	Carbyne bundles for a lithium-ion-battery anode. Journal of the Korean Physical Society, 2013, 63, 1014-1018.	0.3	5
66	Multilayer Graphynes for Lithium Ion Battery Anode. Journal of Physical Chemistry C, 2013, 117, 6919-6923.	1.5	189
67	Exotic Geometrical and Electronic Properties in Hydrogenated Graphyne. Journal of Physical Chemistry C, 2013, 117, 11960-11967.	1.5	41
68	Graphdiyne as a high-capacity lithium ion battery anode material. Applied Physics Letters, 2013, 103, .	1.5	104
69	Thermodynamically Stable Calcium-Decorated Graphyne as a Hydrogen Storage Medium. Journal of Physical Chemistry C, 2012, 116, 20220-20224.	1.5	147
70	High electric field enhancement near electron-doped semiconductor nanoribbons. Chemical Physics Letters, 2012, 546, 99-105.	1.2	0
71	Defect and impurity properties of hexagonal boron nitride: A first-principles calculation. Physical Review B, 2012, 86, .	1.1	187
72	Effects of defects and non-coordinating molecular overlayers on the work function of graphene and energy-level alignment with organic molecules. Carbon, 2012, 50, 851-856.	5.4	20

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73	Edge stability of boron nitride nanoribbons and its application in designing hybrid BNC structures. Nano Research, 2012, 5, 62-72.	5.8	62
74	Gate-controlled ionization and screening of cobalt adatoms on a graphene surface. Nature Physics, 2011, 7, 43-47.	6.5	233
75	Calcium-Decorated Carbyne Networks as Hydrogen Storage Media. Nano Letters, 2011, 11, 2660-2665.	4.5	98
76	Chemical engineering of adamantane by lithium functionalization: A first-principles density functional theory study. Physical Review B, 2011, 83, .	1.1	17
77	Enhancement of adsorption on a boron-doped carbon system for hydrogen storage. Solid State Communications, 2010, 150, 1959-1962.	0.9	10
78	Beryllium-dihydrogen complexes on nanostructures. Applied Physics Letters, 2010, 96, .	1.5	14
79	ReleasingH2molecules with a partial pressure difference without the use of temperature. Physical Review B, 2010, 82, .	1.1	3
80	Selective functionalization of halogens on zigzag graphene nanoribbons: A route to the separation of zigzag graphene nanoribbons. Applied Physics Letters, 2010, 97, 233101.	1.5	23
81	Preferential functionalization on zigzag graphene nanoribbons: first-principles calculations. Journal of Physics Condensed Matter, 2010, 22, 352205.	0.7	11
82	Intrinsic half-metallic BNâ€“C nanotubes. Applied Physics Letters, 2010, 97, 043115.	1.5	54
83	Ab initio study of beryllium-decorated fullerenes for hydrogen storage. Journal of Applied Physics, 2010, 107, .	1.1	22
84	Calcium-Decorated Graphene-Based Nanostructures for Hydrogen Storage. Nano Letters, 2010, 10, 793-798.	4.5	331
85	Calcium-decorated carbon nanotubes for high-capacity hydrogen storage: First-principles calculations. Physical Review B, 2009, 80, .	1.1	148
86	Titanium-functional group complexes for high-capacity hydrogen storage materials. Solid State Communications, 2008, 146, 431-434.	0.9	30
87	Hydrogen storage using functionalized saturated hydrocarbons. Solid State Communications, 2008, 147, 419-422.	0.9	14
88	Hydrogen storage in alkali-metal-decorated organic molecules. Applied Physics Letters, 2008, 93, 063107.	1.5	28
89	Room-temperature dissociative hydrogen chemisorption on boron-doped fullerenes. Physical Review B, 2008, 77, .	1.1	19
90	Ab initiostudy of dihydrogen binding in metal-decorated polyacetylene for hydrogen storage. Physical Review B, 2007, 76, .	1.1	104

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91	Combinatorial Search for Optimal Hydrogen-Storage Nanomaterials Based on Polymers. Physical Review Letters, 2006, 97, 056104.	2.9	192