

Geunsik Lee

List of Publications by Year in descending order

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117
papers

6,722
citations

109321

35
h-index

62596

80
g-index

124
all docs

124
docs citations

124
times ranked

11434
citing authors

#	ARTICLE	IF	CITATIONS
1	Geomimetic Hydrothermal Synthesis of Polyimide-Based Covalent Organic Frameworks. <i>Angewandte Chemie</i> , 2022, 134, .	2.0	5
2	Geomimetic Hydrothermal Synthesis of Polyimide-Based Covalent Organic Frameworks. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	30
3	Controlling interlayer magnetic coupling in the two-dimensional magnet Fe_2Se_2 . <i>Physical Review B</i> , 2022, 105, .	3.2	3
4	Innentitelbild: Geomimetic Hydrothermal Synthesis of Polyimide-Based Covalent Organic Frameworks (<i>Angew. Chem.</i> 4/2022). <i>Angewandte Chemie</i> , 2022, 134, .	2.0	0
5	Machine learning assisted high-throughput screening of transition metal single atom based superb hydrogen evolution electrocatalysts. <i>Journal of Materials Chemistry A</i> , 2022, 10, 6679-6689.	10.3	74
6	Dissolving Diamond: Kinetics of the Dissolution of (100) and (110) Single Crystals in Nickel and Cobalt Films. <i>Chemistry of Materials</i> , 2022, 34, 2599-2611.	6.7	3
7	Enhanced band-filling effect in halide perovskites via hydrophobic conductive linkers. <i>Cell Reports Physical Science</i> , 2022, 3, 100800.	5.6	3
8	Solar-to-hydrogen peroxide conversion of photocatalytic carbon dots with anthraquinone: Unveiling the dual role of surface functionalities. <i>Applied Catalysis B: Environmental</i> , 2022, 312, 121379.	20.2	28
9	A single-atom vanadium-doped 2D semiconductor platform for attomolar-level molecular sensing. <i>Journal of Materials Chemistry A</i> , 2022, 10, 13298-13304.	10.3	12
10	Unveiling the Role of Charge Transfer in Enhanced Electrochemical Nitrogen Fixation at Single-Atom Catalysts on BX Sheets (X = As, P, Sb). <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 4530-4537.	4.6	29
11	Fe- and Co-based magnetic tunnel junctions with AlN and ZnO spacers. <i>Physical Review B</i> , 2022, 105, .	3.2	3
12	Molecularly Engineered Carbon Platform To Anchor Edge-Hosted Single-Atomic N/C (M = Fe, Co, Ni) Tj ETQq0,0,0 rgBT /Overlock 1	11.2	36
13	Conformational heterogeneity of molecules physisorbed on a gold surface at room temperature. <i>Nature Communications</i> , 2022, 13, .	12.8	7
14	Unprecedented electrocatalytic oxygen evolution performances by cobalt-incorporated molybdenum carbide microflowers with controlled charge re-distribution. <i>Journal of Materials Chemistry A</i> , 2021, 9, 1770-1783.	10.3	13
15	Facile room-temperature self-assembly of extended cation-free guanine-quartet network on Mo-doped Au(111) surface. <i>Nanoscale Advances</i> , 2021, 3, 3867-3874.	4.6	2
16	The impact of molecular orientation on carrier transfer characteristics at a phthalocyanine and halide perovskite interface. <i>RSC Advances</i> , 2021, 11, 31776-31782.	3.6	6
17	Tip-Induced Nano-Engineering of Strain, Bandgap, and Exciton Funneling in 2D Semiconductors. <i>Advanced Materials</i> , 2021, 33, e2008234.	21.0	44
18	Graphene Antiadhesion Layer for the Effective Peel-and-Pick Transfer of Metallic Electrodes toward Flexible Electronics. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 22000-22008.	8.0	2

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19	First principles and machine learning based superior catalytic activities and selectivities for N_2 reduction in MBenes, defective 2D materials and 2D π -conjugated polymer-supported single atom catalysts. <i>Journal of Materials Chemistry A</i> , 2021, 9, 9203-9213.	10.3	67
20	Triboelectric Charge-Driven Enhancement of the Output Voltage of BiSbTe-Based Thermoelectric Generators. <i>ACS Energy Letters</i> , 2021, 6, 1095-1103.	17.4	18
21	Late Transition Metal Doped MXenes Showing Superb Bifunctional Electrocatalytic Activities for Water Splitting via Distinctive Mechanistic Pathways. <i>Advanced Energy Materials</i> , 2021, 11, 2102388.	19.5	73
22	Edge functionalized graphene nanoribbons with tunable band edges for carrier transport interlayers in organic-inorganic perovskite solar cells. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 2955-2962.	2.8	4
23	Transport gaps in ideal zigzag-edge graphene nanoribbons with chemical edge disorder. <i>Applied Surface Science</i> , 2020, 512, 144714.	6.1	5
24	Immobilizing single atom catalytic sites onto highly reduced carbon hosts: Fe $_4$ /CNT as a durable oxygen reduction catalyst for Na-air batteries. <i>Journal of Materials Chemistry A</i> , 2020, 8, 18891-18902.	10.3	31
25	Unveiling 79-Year-Old Ixene and Its BN-Doped Derivative. <i>Angewandte Chemie</i> , 2020, 132, 15001-15005.	2.0	7
26	Unveiling 79-Year-Old Ixene and Its BN-Doped Derivative. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 14891-14895.	13.8	29
27	Zwitterionic Conjugated Surfactant Functionalization of Graphene with pH-Independent Dispersibility: An Efficient Electron Mediator for the Oxygen Evolution Reaction in Acidic Media. <i>Small</i> , 2020, 16, 1906635.	10.0	8
28	Ultrasensitive Plasmon-Free Surface-Enhanced Raman Spectroscopy with Femtomolar Detection Limit from 2D van der Waals Heterostructure. <i>Nano Letters</i> , 2020, 20, 1620-1630.	9.1	60
29	A new class of ferromagnetic semiconductor: Copper molybdate organic-inorganic compound with phenanthroline organic linkers. <i>Journal of Magnetism and Magnetic Materials</i> , 2020, 508, 166881.	2.3	2
30	A high performance N-doped graphene nanoribbon based spintronic device applicable with a wide range of adatoms. <i>Nanoscale Advances</i> , 2020, 2, 5905-5911.	4.6	10
31	Homogeneous Li deposition through the control of carbon dot-assisted Li-dendrite morphology for high-performance Li-metal batteries. <i>Journal of Materials Chemistry A</i> , 2019, 7, 20325-20334.	10.3	35
32	An effective approach to realize graphene based p-n junctions via adsorption of donor and acceptor molecules. <i>Carbon</i> , 2019, 153, 525-530.	10.3	6
33	Multiferroicity in atomic van der Waals heterostructures. <i>Nature Communications</i> , 2019, 10, 2657.	12.8	224
34	Band gap tuning and excitonic effect in chloro-fluorinated graphene. <i>Surface Science</i> , 2019, 686, 39-44.	1.9	11
35	Electrocatalytic property of water oxidation reaction depends on charging state of intermediates on Ag-M (M = Fe, Co, Ni, Cu) in alkaline media. <i>International Journal of Hydrogen Energy</i> , 2019, 44, 5863-5871.	7.1	5
36	Signature of multilayer growth of 2D layered Bi $_2$ Se $_3$ through heteroatom-assisted step-edge barrier reduction. <i>Npj 2D Materials and Applications</i> , 2019, 3, .	7.9	1

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37	A New Perspective on the Role of A-Site Cations in Perovskite Solar Cells. <i>Advanced Energy Materials</i> , 2018, 8, 1702898.	19.5	47
38	Oxygen-induced defects at the lead halide perovskite/graphene oxide interfaces. <i>Journal of Materials Chemistry A</i> , 2018, 6, 1423-1442.	10.3	26
39	Temperature induced crossing in the optical bandgap of mono and bilayer MoS ₂ on SiO ₂ . <i>Scientific Reports</i> , 2018, 8, 5380.	3.3	5
40	Sulfur-vacancy-dependent geometric and electronic structure of bismuth adsorbed on MoS_2 . <i>Physical Review B</i> , 2018, 97, .	3.2	4
41	Substitutional Growth of Methylammonium Lead Iodide Perovskites in Alcohols. <i>Advanced Energy Materials</i> , 2018, 8, 1701726.	19.5	28
42	Organic cation steered interfacial electron transfer within organic-inorganic perovskite solar cells. <i>Journal of Materials Chemistry A</i> , 2018, 6, 4305-4312.	10.3	15
43	La-doped BaSnO ₃ electron transport layer for perovskite solar cells. <i>Journal of Materials Chemistry A</i> , 2018, 6, 23071-23077.	10.3	37
44	Unified low-energy effective Hamiltonian and the band topology of p-block square-net layer derivatives. <i>Physical Review B</i> , 2018, 98, .	3.2	6
45	A highly hydrophobic fluorographene-based system as an interlayer for electron transport in organic-inorganic perovskite solar cells. <i>Journal of Materials Chemistry A</i> , 2018, 6, 18635-18640.	10.3	20
46	Perovskite Solar Cells: A New Perspective on the Role of A-Site Cations in Perovskite Solar Cells (Adv.) <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf</i>	19.5	1
47	Multicomponent electrocatalyst with ultralow Pt loading and high hydrogen evolution activity. <i>Nature Energy</i> , 2018, 3, 773-782.	39.5	542
48	Rashba-Dresselhaus Effect in Inorganic/Organic Lead Iodide Perovskite Interfaces. <i>ACS Energy Letters</i> , 2018, 3, 1294-1300.	17.4	36
49	Effects of contact material on complex excitonic behaviour of monolayer MoS ₂ . <i>Optical Materials</i> , 2018, 84, 870-873.	3.6	4
50	Electronic transport across metal-graphene edge contact. <i>2D Materials</i> , 2017, 4, 025033.	4.4	4
51	Density Functional Theory (DFT) Calculations for Oxygen Reduction Reaction Mechanisms on Metal-, Nitrogen- co-doped Graphene (M-N ₂ -G (M = Ti, Cu, Mo, Nb and Ru)) Electrocatalysts. <i>Electrochimica Acta</i> , 2017, 228, 619-627.	5.2	29
52	Two-Dimensional Excitonic Photoluminescence in Graphene on a Cu Surface. <i>ACS Nano</i> , 2017, 11, 3207-3212.	14.6	11
53	Adsorption of Carbon Tetrahalides on Coronene and Graphene. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14968-14974.	3.1	11
54	Efficient CO Oxidation by 50-Facet Cu ₂ O Nanocrystals Coated with CuO Nanoparticles. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 2495-2499.	8.0	31

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55	Screening of Oxygen-Reduction-Reaction-Efficient Electrocatalysts Based on Ag ⁿ (M = 3d, 4d, and 5d) Tj ETQq1 1 0.784314 rgBT 1874-1881.	5.1	13
56	Effects of impurity adsorption on topological surface states of Bi ₂ Te ₃ . Europhysics Letters, 2017, 119, 47001.	2.0	3
57	Ferromagnetism in Monatomic Chains: Spin-Dependent Bandwidth Narrowing/Broadening. Journal of Physical Chemistry C, 2017, 121, 20994-21000.	3.1	8
58	Anomalous Ambipolar Transport of Organic Semiconducting Crystals via Control of Molecular Packing Structures. ACS Applied Materials & Interfaces, 2017, 9, 27839-27846.	8.0	10
59	Lower Electric Field-Driven Magnetic Phase Transition and Perfect Spin Filtering in Graphene Nanoribbons by Edge Functionalization. Journal of Physical Chemistry Letters, 2016, 7, 5049-5055.	4.6	39
60	Integrative Approach toward Uncovering the Origin of Photoluminescence in Dual Heteroatom-Doped Carbon Nanodots. Chemistry of Materials, 2016, 28, 6840-6847.	6.7	128
61	Orbital hybridization mechanism for the enhanced photoluminescence in edge-functionalized sp ² carbon clusters. Carbon, 2016, 109, 418-427.	10.3	8
62	Oxygen Reduction Reaction Mechanisms on Al-Doped X-Graphene (X = N, P, and S) Catalysts in Acidic Medium: A Comparative DFT Study. Journal of Physical Chemistry C, 2016, 120, 26435-26441.	3.1	30
63	Electron Transport in Graphene Nanoribbon Field-Effect Transistor under Bias and Gate Voltages: Isochemical Potential Approach. Journal of Physical Chemistry Letters, 2016, 7, 2478-2482.	4.6	33
64	APEX Fingerprinting Reveals the Subcellular Localization of Proteins of Interest. Cell Reports, 2016, 15, 1837-1847.	6.4	153
65	Real-Time Propagation via Time-Dependent Density Functional Theory Plus the Hubbard U Potential for Electron-Atom Coupled Dynamics Involving Charge Transfer. Journal of Chemical Theory and Computation, 2016, 12, 201-208.	5.3	23
66	Surface-Effect-Induced Optical Bandgap Shrinkage in GaN Nanotubes. Nano Letters, 2015, 15, 4472-4476.	9.1	21
67	Graphene Edges and Beyond: Temperature-Driven Structures and Electromagnetic Properties. ACS Nano, 2015, 9, 4669-4674.	14.6	31
68	Geometrical and Electronic Characteristics of Au _n O ₂ (n = 7). Journal of Physical Chemistry C, 2015, 119, 14383-14391.	3.1	13
69	Tailoring Electronic and Magnetic Properties of MoS ₂ Nanotubes. Journal of Physical Chemistry C, 2015, 119, 6405-6413.	3.1	40
70	Grain Boundary Effect on Electrical Transport Properties of Graphene. Journal of Physical Chemistry C, 2014, 118, 2338-2343.	3.1	71
71	Spin-induced band modifications of graphene through intercalation of magnetic iron atoms. Nanoscale, 2014, 6, 3824-3829.	5.6	51
72	Density Functional Theory Based Study of Molecular Interactions, Recognition, Engineering, and Quantum Transport in π Molecular Systems. Accounts of Chemical Research, 2014, 47, 3321-3330.	15.6	54

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73	Two Dimensional Molecular Electronics Spectroscopy for Molecular Fingerprinting, DNA Sequencing, and Cancerous DNA Recognition. ACS Nano, 2014, 8, 1827-1833.	14.6	65
74	Inverse Transfer Method Using Polymers with Various Functional Groups for Controllable Graphene Doping. ACS Nano, 2014, 8, 7968-7975.	14.6	26
75	AEMnSb ₂ (AE=Sr, Ba): a new class of Dirac materials. Journal of Physics Condensed Matter, 2014, 26, 042201.	1.8	57
76	Valley-Polarized Interlayer Conduction of Anisotropic Dirac Fermions in $SrMnBi_2$. Physical Review Letters, 2014, 113, 156602.	7.8	48
77	Spectroscopic evaluation of out-of-plane surface vibration bands from surface functionalization of graphite oxide by fluorination. Carbon, 2014, 77, 577-591.	10.3	11
78	Substrate-Induced Solvent Intercalation for Stable Graphene Doping. ACS Nano, 2013, 7, 1155-1162.	14.6	54
79	Noncovalent Functionalization with Alkali Metal to Separate Semiconducting from Metallic Carbon Nanotubes: A Theoretical Study. Journal of Physical Chemistry C, 2013, 117, 4309-4313.	3.1	13
80	Anisotropic Dirac electronic structures of $MnBi_2A$.		

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91	Small anisotropy in iron-based superconductors induced by electron correlation. Physical Review B, 2011, 84, .	3.2	7
92	Origin of HfO ₂ /GaAs interface states and interface passivation: A first principles study. Applied Surface Science, 2010, 256, 6569-6573.	6.1	30
93	Unusual infrared-absorption mechanism in thermally reduced graphene oxide. Nature Materials, 2010, 9, 840-845.	27.5	724
94	Isotope Effect on the Thermal Conductivity of Graphene. Journal of Nanomaterials, 2010, 2010, 1-5.	2.7	45
95	First-principles study of GaAs(001)- $\sqrt{2}(\sqrt{2}\times\sqrt{2})$ surface oxidation and passivation with H, Cl, S, F, and GaO. Journal of Applied Physics, 2010, 107, .	2.5	74
96	First-principles study of metal-graphene interfaces. Journal of Applied Physics, 2010, 108, .	2.5	358
97	First-Principles and Quantum Transport Studies of Metal-Graphene End Contacts. Materials Research Society Symposia Proceedings, 2010, 1259, 1.	0.1	2
98	The Role of Intercalated Water in Multilayered Graphene Oxide. ACS Nano, 2010, 4, 5861-5868.	14.6	359
99	Materials Science of Graphene for Novel Device Applications. ECS Transactions, 2009, 19, 185-199.	0.5	2
100	First-Principles study of HfO ₂ /GaAs interface passivation by Si and Ge. Materials Research Society Symposia Proceedings, 2009, 1155, 1.	0.1	0
101	Electronic structures of zigzag graphene nanoribbons with edge hydrogenation and oxidation. Physical Review B, 2009, 79, .	3.2	239
102	Ozone Adsorption on Graphene: Ab Initio Study and Experimental Validation. Journal of Physical Chemistry C, 2009, 113, 14225-14229.	3.1	170
103	Nanoclusters of Group-III Metal Atoms on Si(111)- $\sqrt{7}\times\sqrt{7}$. Journal of Computational and Theoretical Nanoscience, 2009, 6, 1311-1319.	0.4	2
104	Self-trapping nature of Tl nanoclusters on the Si(111)- $\sqrt{7}\times\sqrt{7}$ surface. New Journal of Physics, 2008, 10, 053013.	2.9	2
105	Ab initio studies of structural and electronic properties of the crystalline Ge_2 . Physical Review B, 2008, 77, .	3.2	30
106	Ab initio study of thallium nanoclusters on Si surface. Physical Review B, 2007, 76, .	3.2	19
107	Adsorption energies of Al, Ga, In, Tl on Si(111)-. Computer Physics Communications, 2007, 177, 44.	7.5	2
108	Origin of unusual work function change upon forming Tl nanoclusters on Si(111)- 7×7 surface. Applied Physics A: Materials Science and Processing, 2007, 89, 431-435.	2.3	5

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109	Electronic structure and optical absorption spectra of CdSe covered with ZnSe and ZnS epilayers. Solid State Communications, 2006, 137, 332-337.	1.9	9
110	Ab initio α phase diagram of NaBH ₄ . Solid State Communications, 2006, 139, 516-521.	1.9	23
111	Theoretical study of the electronic structure and hydrogen adsorption properties in B2-TiFe thin films with Pd coating. International Journal of Hydrogen Energy, 2004, 29, 87-92.	7.1	13
112	Numerical verification of topological crossings in band structure of solids. Journal of Physics Condensed Matter, 2003, 15, 2005-2016.	1.8	5
113	Surface electronic structure of Ti-based transition metal alloys. Physical Review B, 2002, 65, .	3.2	14
114	The electronic properties of FeCo, Ni ₃ Mn and Ni ₃ Fe at the order-disorder transition. Physica B: Condensed Matter, 2002, 322, 236-247.	2.7	25
115	The adsorption of hydrogen on B2 TiFe surfaces. International Journal of Hydrogen Energy, 2002, 27, 403-412.	7.1	34
116	Electronic structure of binary and ternary Ti-based shape-memory alloys. Solid State Communications, 2001, 119, 619-623.	1.9	21
117	Optical properties of TiNi, TiCo and TiFe thin films. Physica B: Condensed Matter, 2001, 304, 186-192.	2.7	6