

# Geunsik Lee

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/3582112/publications.pdf>

Version: 2024-02-01

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	The Role of Oxygen during Thermal Reduction of Graphene Oxide Studied by Infrared Absorption Spectroscopy. Journal of Physical Chemistry C, 2011, 115, 19761-19781.	3.1	776
2	Unusual infrared-absorption mechanism in thermally reduced graphene oxide. Nature Materials, 2010, 9, 840-845.	27.5	724
3	Multicomponent electrocatalyst with ultralow Pt loading and high hydrogen evolution activity. Nature Energy, 2018, 3, 773-782.	39.5	542
4	The Role of Intercalated Water in Multilayered Graphene Oxide. ACS Nano, 2010, 4, 5861-5868.	14.6	359
5	First-principles study of metal-graphene interfaces. Journal of Applied Physics, 2010, 108, .	2.5	358
6	Electronic structures of zigzag graphene nanoribbons with edge hydrogenation and oxidation. Physical Review B, 2009, 79, .	3.2	239
7	Anisotropic Dirac Fermions in a Bi Square Net of $\text{SrMnBi}_2$ . Physical Review Letters, 2011, 107, 126402.	7.8	230
8	Multiferroicity in atomic van der Waals heterostructures. Nature Communications, 2019, 10, 2657.	12.8	224
9	Thermal transport in graphene and effects of vacancy defects. Physical Review B, 2011, 84, .	3.2	199
10	Ozone Adsorption on Graphene: Ab Initio Study and Experimental Validation. Journal of Physical Chemistry C, 2009, 113, 14225-14229.	3.1	170
11	APEX Fingerprinting Reveals the Subcellular Localization of Proteins of Interest. Cell Reports, 2016, 15, 1837-1847.	6.4	153
12	Integrative Approach toward Uncovering the Origin of Photoluminescence in Dual Heteroatom-Doped Carbon Nanodots. Chemistry of Materials, 2016, 28, 6840-6847.	6.7	128
13	Atomic Layer Deposition of Dielectrics on Graphene Using Reversibly Physisorbed Ozone. ACS Nano, 2012, 6, 2722-2730.	14.6	115
14	Anisotropic Dirac electronic structures of $\text{MnBiA}$ .		

#	ARTICLE	IF	CITATIONS
19	Grain Boundary Effect on Electrical Transport Properties of Graphene. Journal of Physical Chemistry C 2014, 118, 2338-2343. Orbital Selective Fermi Surface Shifts and Mechanism of High	3.1	71
20	Superconductivity in Correlated		

#	ARTICLE	IF	CITATIONS
37	Molecularly Engineered Carbon Platform To Anchor Edge-Hosted Single-Atomic M <sup>n</sup> /C (M = Fe, Co, Ni). <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 11.2	11.2	36
38	Reparameterization of the REBO-CHO potential for graphene oxide molecular dynamics simulations. <i>Physical Review B</i> , 2011, 84, .	3.2	35
39	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
40	The adsorption of hydrogen on B2 TiFe surfaces. <i>International Journal of Hydrogen Energy</i> , 2002, 27, 403-412.	7.1	34
41	Electron Transport in Graphene Nanoribbon Field-Effect Transistor under Bias and Gate Voltages: Isochemical Potential Approach. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2478-2482.	4.6	33
42	Graphene Edges and Beyond: Temperature-Driven Structures and Electromagnetic Properties. <i>ACS Nano</i> , 2015, 9, 4669-4674.	14.6	31
43	Efficient CO Oxidation by 50-Facet Cu <sub>2</sub> O Nanocrystals Coated with CuO Nanoparticles. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 2495-2499.	8.0	31
44	Immobilizing single atom catalytic sites onto highly reduced carbon hosts: Fe <sub>4</sub> /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
45	<i>Ab initio</i> studies of structural and electronic properties of the crystalline $Ge_2$ . <i>Physical Review B</i> , 2008, 77, .	3.2	30
46	Origin of HfO <sub>2</sub> /GaAs interface states and interface passivation: A first principles study. <i>Applied Surface Science</i> , 2010, 256, 6569-6573.	6.1	30
47	Oxygen Reduction Reaction Mechanisms on Al-Doped X-Graphene (X = N, P, and S) Catalysts in Acidic Medium: A Comparative DFT Study. <i>Journal of Physical Chemistry C</i> , 2016, 120, 26435-26441.	3.1	30
48	Geomimetic Hydrothermal Synthesis of Polyimide-Based Covalent Organic Frameworks. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	30
49	Density Functional Theory (DFT) Calculations for Oxygen Reduction Reaction Mechanisms on Metal-, Nitrogen- co-doped Graphene (M-N <sub>2</sub> -G (M = Ti, Cu, Mo, Nb and Ru)) Electrocatalysts. <i>Electrochimica Acta</i> , 2017, 228, 619-627.	5.2	29
50	Unveiling 79-year-old Ixene and Its BN-Doped Derivative. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 14891-14895.	13.8	29
51	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
52	Theoretical Study of the Electron Transport in Graphene with Vacancy and Residual Oxygen Defects after High-Temperature Reduction. <i>Journal of Physical Chemistry C</i> , 2011, 115, 9719-9725.	3.1	28
53	Substitutional Growth of Methylammonium Lead Iodide Perovskites in Alcohols. <i>Advanced Energy Materials</i> , 2018, 8, 1701726.	19.5	28
54	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

#	ARTICLE	IF	CITATIONS
55	Inverse Transfer Method Using Polymers with Various Functional Groups for Controllable Graphene Doping. ACS Nano, 2014, 8, 7968-7975.	14.6	26
56	Oxygen-induced defects at the lead halide perovskite/graphene oxide interfaces. Journal of Materials Chemistry A, 2018, 6, 1423-1442.	10.3	26
57	The electronic properties of FeCo, Ni <sub>3</sub> Mn and Ni <sub>3</sub> Fe at the order-disorder transition. Physica B: Condensed Matter, 2002, 322, 236-247.	2.7	25
58	Ab initio phase diagram of NaBH <sub>4</sub> . Solid State Communications, 2006, 139, 516-521.	1.9	23
59	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
60	Electronic structure of binary and ternary Ti-based shape-memory alloys. Solid State Communications, 2001, 119, 619-623.	1.9	21
61	Surface-Effect-Induced Optical Bandgap Shrinkage in GaN Nanotubes. Nano Letters, 2015, 15, 4472-4476.	9.1	21
62	A highly hydrophobic fluorographene-based system as an interlayer for electron transport in organic-inorganic perovskite solar cells. Journal of Materials Chemistry A, 2018, 6, 18635-18640.	10.3	20
63	Ab initio study of thallium nanoclusters on Si. Physical Review B, 2007, 76, .	3.2	19
64	Triboelectric Charge-Driven Enhancement of the Output Voltage of BiSbTe-Based Thermoelectric Generators. ACS Energy Letters, 2021, 6, 1095-1103.	17.4	18
65	Organic cation steered interfacial electron transfer within organic-inorganic perovskite solar cells. Journal of Materials Chemistry A, 2018, 6, 4305-4312.	10.3	15
66	Surface electronic structure of Ti-based transition metal alloys. Physical Review B, 2002, 65, .	3.2	14
67	Theoretical study of the electronic structure and hydrogen adsorption properties in B <sub>2</sub> -TiFe thin films with Pd coating. International Journal of Hydrogen Energy, 2004, 29, 87-92.	7.1	13
68	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
69	Geometrical and Electronic Characteristics of Au <sub>n</sub> O <sub>2</sub> (n = 2-7). Journal of Physical Chemistry C, 2015, 119, 14383-14391.	3.1	13
70	Screening of Oxygen-Reduction-Reaction-Efficient Electrocatalysts Based on Ag <sub>n</sub> (M = 3d, 4d, and 5d) Tj ETQq0 0 0 rgBT /Overlock 1874-1881.	5.1	13
71	Unprecedented electrocatalytic oxygen evolution performances by cobalt-incorporated molybdenum carbide microflowers with controlled charge re-distribution. Journal of Materials Chemistry A, 2021, 9, 1770-1783.	10.3	13
72	A single-atom vanadium-doped 2D semiconductor platform for attomolar-level molecular sensing. Journal of Materials Chemistry A, 2022, 10, 13298-13304.	10.3	12

#	ARTICLE	IF	CITATIONS
73	First-principles study of GaAs(001)- $\sqrt{2}(\sqrt{2}\times\sqrt{2})$ surface oxidation. <i>Microelectronic Engineering</i> , 2011, 88, 3419-3423.	2.4	11
74	Spectroscopic evaluation of out-of-plane surface vibration bands from surface functionalization of graphite oxide by fluorination. <i>Carbon</i> , 2014, 77, 577-591.	10.3	11
75	Two-Dimensional Excitonic Photoluminescence in Graphene on a Cu Surface. <i>ACS Nano</i> , 2017, 11, 3207-3212.	14.6	11
76	Adsorption of Carbon Tetrahalides on Coronene and Graphene. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14968-14974.	3.1	11
77	Band gap tuning and excitonic effect in chloro- $\alpha$ -fluorinated graphene. <i>Surface Science</i> , 2019, 686, 39-44.	1.9	11
78	Anomalous Ambipolar Transport of Organic Semiconducting Crystals via Control of Molecular Packing Structures. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 27839-27846.	8.0	10
79	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
80	Electronic structure and optical absorption spectra of CdSe covered with ZnSe and ZnS epilayers. <i>Solid State Communications</i> , 2006, 137, 332-337.	1.9	9
81	Controlling interlayer magnetic coupling in the two-dimensional magnet $\text{Fe}_3\text{Ge}_2\text{Te}_5$ . <i>Physical Review B</i> , 2022, 105, .	8.3	9
82	Orbital hybridization mechanism for the enhanced photoluminescence in edge-functionalized sp <sup>2</sup> carbon clusters. <i>Carbon</i> , 2016, 109, 418-427.	10.3	8
83	Ferromagnetism in Monatomic Chains: Spin-Dependent Bandwidth Narrowing/Broadening. <i>Journal of Physical Chemistry C</i> , 2017, 121, 20994-21000.	3.1	8
84	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
85	Small anisotropy in iron-based superconductors induced by electron correlation. <i>Physical Review B</i> , 2011, 84, .	3.2	7
86	Unveiling 79-Year-Old Ixene and Its BN-Doped Derivative. <i>Angewandte Chemie</i> , 2020, 132, 15001-15005.	2.0	7
87	Conformational heterogeneity of molecules physisorbed on a gold surface at room temperature. <i>Nature Communications</i> , 2022, 13, .	12.8	7
88	Optical properties of TiNi, TiCo and TiFe thin films. <i>Physica B: Condensed Matter</i> , 2001, 304, 186-192.	2.7	6
89	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
90	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

#	ARTICLE	IF	CITATIONS
91	The impact of molecular orientation on carrier transfer characteristics at a phthalocyanine and halide perovskite interface. RSC Advances, 2021, 11, 31776-31782.	3.6	6
92	Numerical verification of topological crossings in band structure of solids. Journal of Physics Condensed Matter, 2003, 15, 2005-2016.	1.8	5
93	Origin of unusual work function change upon forming Tl nanoclusters on Si(111)-7x7 surface. Applied Physics A: Materials Science and Processing, 2007, 89, 431-435.	2.3	5
94	Temperature induced crossing in the optical bandgap of mono and bilayer MoS2 on SiO2. Scientific Reports, 2018, 8, 5380.	3.3	5
95	Electrocatalytic property of water oxidation reaction depends on charging state of intermediates on Ag-M (M = Fe, Co, Ni, Cu) in alkaline media. International Journal of Hydrogen Energy, 2019, 44, 5863-5871.	7.1	5
96	Transport gaps in ideal zigzag-edge graphene nanoribbons with chemical edge disorder. Applied Surface Science, 2020, 512, 144714.	6.1	5
97	Geomimetic Hydrothermal Synthesis of Polyimide-Based Covalent Organic Frameworks. Angewandte Chemie, 2022, 134, .	2.0	5
98	Electronic transport across metal-graphene edge contact. 2D Materials, 2017, 4, 025033.	4.4	4
99	Sulfur-vacancy-dependent geometric and electronic structure of bismuth adsorbed on $\text{MoS}_2$ . Physical Review B, 2018, 97, .	3.2	4
100	Effects of contact material on complex excitonic behaviour of monolayer MoS2. Optical Materials, 2018, 84, 870-873.	3.6	4
101	Edge functionalized graphene nanoribbons with tunable band edges for carrier transport interlayers in organic-inorganic perovskite solar cells. Physical Chemistry Chemical Physics, 2020, 22, 2955-2962.	2.8	4
102	Effects of impurity adsorption on topological surface states of Bi <sub>2</sub> Te <sub>3</sub> . Europhysics Letters, 2017, 119, 47001.	2.0	3
103	Dissolving Diamond: Kinetics of the Dissolution of (100) and (110) Single Crystals in Nickel and Cobalt Films. Chemistry of Materials, 2022, 34, 2599-2611.	6.7	3
104	Enhanced band-filling effect in halide perovskites via hydrophobic conductive linkers. Cell Reports Physical Science, 2022, 3, 100800.	5.6	3
105	Fe- and Co-based magnetic tunnel junctions with AlN and ZnO spacers. Physical Review B, 2022, 105, .	3.2	3
106	Adsorption energies of Al, Ga, In, Tl on Si(111)-. Computer Physics Communications, 2007, 177, 44.	7.5	2
107	Self-trapping nature of Tl nanoclusters on the Si(111)-7x7 surface. New Journal of Physics, 2008, 10, 053013.	2.9	2
108	Materials Science of Graphene for Novel Device Applications. ECS Transactions, 2009, 19, 185-199.	0.5	2

#	ARTICLE	IF	CITATIONS
109	Nanoclusters of Group-III Metal Atoms on Si(111)-7 Å <sup>2</sup> . Journal of Computational and Theoretical Nanoscience, 2009, 6, 1311-1319.	0.4	2
110	First-Principles and Quantum Transport Studies of Metal-Graphene End Contacts. Materials Research Society Symposia Proceedings, 2010, 1259, 1.	0.1	2
111	A new class of ferromagnetic semiconductor: Copper molybdate organic-inorganic compound with phenanthroline organic linkers. Journal of Magnetism and Magnetic Materials, 2020, 508, 166881.	2.3	2
112	Facile room-temperature self-assembly of extended cation-free guanine-quartet network on Mo-doped Au(111) surface. Nanoscale Advances, 2021, 3, 3867-3874.	4.6	2
113	Graphene Antiadhesion Layer for the Effective Peel-and-Pick Transfer of Metallic Electrodes toward Flexible Electronics. ACS Applied Materials & Interfaces, 2021, 13, 22000-22008.	8.0	2
114	Perovskite Solar Cells: A New Perspective on the Role of A-Site Cations in Perovskite Solar Cells (Adv.) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	19.5	1
115	Signature of multilayer growth of 2D layered Bi <sub>2</sub> Se <sub>3</sub> through heteroatom-assisted step-edge barrier reduction. Npj 2D Materials and Applications, 2019, 3, .	7.9	1
116	First-Principles study of HfO <sub>2</sub> /GaAs interface passivation by Si and Ge. Materials Research Society Symposia Proceedings, 2009, 1155, 1.	0.1	0
117	Innentitelbild: Geomimetic Hydrothermal Synthesis of Polyimide-Based Covalent Organic Frameworks (Angew. Chem. 4/2022). Angewandte Chemie, 2022, 134, .	2.0	0