

Yong-Hoon Kim

List of Publications by Year in descending order

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94
papers

2,845
citations

186265

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docs citations

97
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3787
citing authors

#	ARTICLE	IF	CITATIONS
1	Brain-Inspired Photonic Neuromorphic Devices using Photodynamic Amorphous Oxide Semiconductors and their Persistent Photoconductivity. <i>Advanced Materials</i> , 2017, 29, 1700951.	21.0	346
2	Structures and Properties of Self-Assembled Monolayers of Bistable [2]Rotaxanes on Au (111) Surfaces from Molecular Dynamics Simulations Validated with Experiment. <i>Journal of the American Chemical Society</i> , 2005, 127, 1563-1575.	13.7	202
3	Two-dimensional limit of exchange-correlation energy functional approximations. <i>Physical Review B</i> , 2000, 61, 5202-5211.	3.2	129
4	Excitonic Optical Spectrum of Semiconductors Obtained by Time-Dependent Density-Functional Theory with the Exact-Exchange Kernel. <i>Physical Review Letters</i> , 2002, 89, 096402.	7.8	111
5	Molecular Dynamics Simulation of Amphiphilic Bistable [2]Rotaxane Langmuir Monolayers at the Air/Water Interface. <i>Journal of the American Chemical Society</i> , 2005, 127, 14804-14816.	13.7	102
6	Modulation of the Electronic Properties of MXene (Ti ₃ C ₂ T _x) via Surface-Covalent Functionalization with Diazonium. <i>ACS Nano</i> , 2021, 15, 1388-1396.	14.6	100
7	Extremely Large Gate Modulation in Vertical Graphene/WSe ₂ Heterojunction Barristor Based on a Novel Transport Mechanism. <i>Advanced Materials</i> , 2016, 28, 5293-5299.	21.0	92
8	Edge-selenated graphene nanoplatelets as durable metal-free catalysts for iodine reduction reaction in dye-sensitized solar cells. <i>Science Advances</i> , 2016, 2, e1501459.	10.3	88
9	Insight into the Microenvironments of the Metal-Ionic Liquid Interface during Electrochemical CO ₂ Reduction. <i>ACS Catalysis</i> , 2018, 8, 2420-2427.	11.2	77
10	Density Functional Theory Studies of the [2]Rotaxane Component of the Stoddart-Heath Molecular Switch. <i>Journal of the American Chemical Society</i> , 2004, 126, 12636-12645.	13.7	74
11	First-Principles Study of the Switching Mechanism of [2]Catenane Molecular Electronic Devices. <i>Physical Review Letters</i> , 2005, 94, 156801.	7.8	72
12	Exact Kohn-Sham exchange kernel for insulators and its long-wavelength behavior. <i>Physical Review B</i> , 2002, 66, .	3.2	71
13	An Optogenetics-Inspired Flexible van der Waals Optoelectronic Synapse and its Application to a Convolutional Neural Network. <i>Advanced Materials</i> , 2021, 33, e2102980.	21.0	65
14	Ab initio study of the effect of water adsorption on the carbon nanotube field-effect transistor. <i>Applied Physics Letters</i> , 2006, 89, 243110.	3.3	63
15	Coherent Lattice Vibrations in Mono- and Few-Layer WSe ₂ . <i>ACS Nano</i> , 2016, 10, 5560-5566.	14.6	62
16	First-principles approach to the charge-transport characteristics of monolayer molecular-electronics devices: Application to hexanedithiolate devices. <i>Physical Review B</i> , 2006, 73, .	3.2	60
17	Ultrafast Discharge/Charge Rate and Robust Cycle Life for High-Performance Energy Storage Using Ultrafine Nanocrystals on the Binder-Free Porous Graphene Foam. <i>Advanced Functional Materials</i> , 2016, 26, 5139-5148.	14.9	53
18	Recent progress in atomistic simulation of electrical current DNA sequencing. <i>Biosensors and Bioelectronics</i> , 2015, 69, 186-198.	10.1	48

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19	HfO ₂ /HfS ₂ hybrid heterostructure fabricated via controllable chemical conversion of two-dimensional HfS ₂ . <i>Nanoscale</i> , 2018, 10, 18758-18766.	5.6	48
20	Density-functional study of small molecules within the Krieger-Li-Iaftrate approximation. <i>Physical Review A</i> , 1999, 60, 3633-3640.	2.5	46
21	Atomic-scale view of stability and degradation of single-crystal MAPbBr ₃ surfaces. <i>Journal of Materials Chemistry A</i> , 2019, 7, 20760-20766.	10.3	46
22	Conformations and charge transport characteristics of biphenyldithiol self-assembled-monolayer molecular electronic devices: A multiscale computational study. <i>Journal of Chemical Physics</i> , 2005, 122, 244703.	3.0	44
23	Origins of genuine Ohmic van der Waals contact between indium and MoS ₂ . <i>Npj 2D Materials and Applications</i> , 2021, 5, .	7.9	43
24	Shell-filling effects and Coulomb degeneracy in planar quantum-dot structures. <i>Physical Review B</i> , 1997, 56, 15752-15759.	3.2	36
25	Direct and defect-assisted electron tunneling through ultrathin SiO_2 from first principles. <i>Physical Review B</i> , 2008, 77, .	3.2	35
26	Electronic and magnetic properties of carbide MXenes—the role of electron correlations. <i>Materials Today Advances</i> , 2021, 9, 100118.	5.2	35
27	One-way multigrid method in electronic-structure calculations. <i>Physical Review B</i> , 2000, 61, 4397-4400.	3.2	32
28	Atomistic mechanisms of codoping-induced p- to n-type conversion in nitrogen-doped graphene. <i>Nanoscale</i> , 2014, 6, 14911-14918.	5.6	30
29	Stretching-Induced Conductance Variations as Fingerprints of Contact Configurations in Single-Molecule Junctions. <i>Journal of the American Chemical Society</i> , 2017, 139, 8286-8294.	13.7	29
30	Epitaxially Self-Assembled Alkane Layers for Graphene Electronics. <i>Advanced Materials</i> , 2017, 29, 1603925.	21.0	24
31	Efficiency of Tunneling in [2]Rotaxane Molecular Electronic Switches. <i>Journal of Physical Chemistry C</i> , 2007, 111, 4831-4837.	3.1	23
32	Quantum interference in DNA bases probed by graphene nanoribbons. <i>Applied Physics Letters</i> , 2013, 103, .	3.3	22
33	Solution-processed oxide semiconductor-based artificial optoelectronic synapse array for spatiotemporal synaptic integration. <i>Journal of Alloys and Compounds</i> , 2021, 857, 158027.	5.5	22
34	Density Functional Theory Study of the Geometry, Energetics, and Reconstruction Process of Si(111) Surfaces. <i>Langmuir</i> , 2005, 21, 12404-12414.	3.5	21
35	Origin and Control of Polyacrylonitrile Alignments on Carbon Nanotubes and Graphene Nanoribbons. <i>Advanced Functional Materials</i> , 2018, 28, 1706970.	14.9	18
36	Raman Scattering Studies of the Structural Phase Transitions in Single-Crystalline CH ₃ NH ₃ PbCl ₃ . <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3773-3781.	4.6	18

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37	Energy States of a Core-Shell Metal Oxide Photocatalyst Enabling Visible Light Absorption and Utilization in Solar-Fuel Conversion of Carbon Dioxide. <i>Advanced Energy Materials</i> , 2016, 6, 1600583.	19.5	17
38	Electrical transport properties of nanoscale devices based on carbon nanotubes. <i>Current Applied Physics</i> , 2009, 9, S7-S11.	2.4	16
39	Conformational and conductance fluctuations in a single-molecule junction: Multiscale computational study. <i>Physical Review B</i> , 2010, 82, .	3.2	16
40	Capacitive energies of quantum dots with hydrogenic impurity. <i>Physical Review B</i> , 1999, 60, 13720-13726.	3.2	15
41	Semimetallicity and Negative Differential Resistance from Hybrid Halide Perovskite Nanowires. <i>Advanced Functional Materials</i> , 2019, 29, 1807620.	14.9	15
42	Surface Termination-Dependent Nanotribological Properties of Single-Crystal MAPbBr ₃ Surfaces. <i>Journal of Physical Chemistry C</i> , 2020, 124, 1484-1491.	3.1	15
43	Strain-Induced Metallization and Defect Suppression at Zipper-like Interdigitated Atomically Thin Interfaces Enabling High-Efficiency Halide Perovskite Solar Cells. <i>ACS Nano</i> , 2021, 15, 1805-1816.	14.6	15
44	Conductance recovery and spin polarization in boron and nitrogen co-doped graphene nanoribbons. <i>Carbon</i> , 2015, 81, 339-346.	10.3	14
45	Quasi-Fermi level splitting in nanoscale junctions from ab initio. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 10142-10148.	7.1	14
46	Anomalous length scaling of carbon nanotube-metal contact resistance: An ab initio study. <i>Applied Physics Letters</i> , 2012, 100, 213113.	3.3	13
47	A facile synthesis of multi metal-doped rectangular ZnO nanocrystals using a nanocrystalline metal-organic framework template. <i>Nanoscale</i> , 2014, 6, 10995-11001.	5.6	13
48	Carbon nanobuds based on carbon nanotube caps: a first-principles study. <i>Nanoscale</i> , 2016, 8, 2343-2349.	5.6	13
49	Highly luminescent blue-emitting CdZnS/ZnS nanorods having electric-field-induced fluorescence switching properties. <i>Journal of Materials Chemistry C</i> , 2017, 5, 2098-2106.	5.5	13
50	MXene Phase with C ₃ Structure Unit: A Family of 2D Electrides. <i>Advanced Functional Materials</i> , 2021, 31, 2100009.	14.9	13
51	All-Inkjet-Printed Vertical Heterostructure for Wafer-Scale Electronics. <i>ACS Nano</i> , 2019, 13, 8213-8221.	14.6	12
52	Atomistics of Asymmetric Lateral Growth of Colloidal Zincblende CdSe Nanoplatelets. <i>Chemistry of Materials</i> , 2021, 33, 4813-4820.	6.7	12
53	Electronic structure of ellipsoidally deformed quantum dots. <i>Journal of Physics Condensed Matter</i> , 2001, 13, 1987-1993.	1.8	11
54	First-principles study of the electrical conductance of telescopically aligned carbon nanotubes. <i>Physical Review B</i> , 2007, 76, .	3.2	11

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55	Charge Transport through Polyene Self-Assembled Monolayers from Multiscale Computer Simulations. <i>Journal of Physical Chemistry B</i> , 2008, 112, 14888-14897.	2.6	11
56	Distinct Mechanisms of DNA Sensing Based on Na ⁺ -Doped Carbon Nanotubes with Enhanced Conductance and Chemical Selectivity. <i>Small</i> , 2014, 10, 774-781.	10.0	11
57	Design and optimization of cobalt-encapsulating vertical graphene nano-hills for hydrogen evolution reaction. <i>Journal of Materials Chemistry A</i> , 2019, 7, 17046-17052.	10.3	11
58	Atomistic mechanisms of seeding promoter-controlled growth of molybdenum disulphide. <i>2D Materials</i> , 2020, 7, 015013.	4.4	11
59	Possible performance improvement in [2]catenane molecular electronic switches. <i>Applied Physics Letters</i> , 2006, 88, 163112.	3.3	9
60	Intrinsically low-resistance carbon nanotube-metal contacts mediated by topological defects. <i>MRS Communications</i> , 2012, 2, 91-96.	1.8	9
61	Prediction of ultra-high ON/OFF ratio nanoelectromechanical switching from covalently-bound C60 chains. <i>Carbon</i> , 2014, 67, 48-57.	10.3	9
62	Nitrogen Doping of Carbon Nanoelectrodes for Enhanced Control of DNA Translocation Dynamics. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 18227-18236.	8.0	9
63	Odd-even phonon transport effects in strained carbon atomic chains bridging graphene nanoribbon electrodes. <i>Carbon</i> , 2019, 142, 107-114.	10.3	9
64	First-principles-derived effective mass approximation for the improved description of quantum nanostructures. <i>JPhys Materials</i> , 2020, 3, 034012.	4.2	9
65	Toward Numerically Accurate First-Principles Calculations of Nano-Device Charge Transport Characteristics: The Case of Alkane Single-Molecule Junctions. <i>Journal of the Korean Physical Society</i> , 2008, 52, 1181-1186.	0.7	9
66	Electrical and Mechanical Switching in a Realistic [2]Rotaxane Device Model. <i>Journal of Nanoscience and Nanotechnology</i> , 2008, 8, 4593-4597.	0.9	8
67	Multi-space Excitation as an Alternative to the Landauer Picture for Nonequilibrium Quantum Transport. <i>Advanced Science</i> , 2020, 7, 2001038.	11.2	8
68	Valley depolarization in monolayer transition-metal dichalcogenides with zone-corner acoustic phonons. <i>Nanoscale</i> , 2020, 12, 22487-22494.	5.6	8
69	Emergence of multiple negative differential transconductance from a WSe ₂ double lateral homojunction platform. <i>Applied Surface Science</i> , 2022, 581, 152396.	6.1	8
70	Gate- versus defect-induced voltage drop and negative differential resistance in vertical graphene heterostructures. <i>Npj Computational Materials</i> , 2022, 8, .	8.7	8
71	Object-oriented construction of a multigrid electronic-structure code with Fortran 90. <i>Computer Physics Communications</i> , 2000, 131, 10-25.	7.5	6
72	Optical excitations of Si by time-dependent density functional theory based on exact-exchange Kohn-Sham band structure. <i>International Journal of Quantum Chemistry</i> , 2003, 91, 257-262.	2.0	6

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73	Metal-Independent Coherent Electron Tunneling through Polymerized Fullerene Chains. Journal of Physical Chemistry C, 2008, 112, 7029-7035.	3.1	6
74	Anomalous transport properties in boron and phosphorus co-doped armchair graphene nanoribbons. Nanotechnology, 2016, 27, 47LT01.	2.6	6
75	Zero power infrared sensing in 2D/3D-assembled heterogeneous graphene/In/InSe/Au. Nanoscale, 2022, 14, 3004-3012.	5.6	6
76	Quantum hybridization negative differential resistance from non-toxic halide perovskite nanowire heterojunctions and its strain control. Nano Convergence, 2022, 9, .	12.1	6
77	Shear-strain-mediated photoluminescence manipulation in two-dimensional transition metal dichalcogenides. 2D Materials, 2022, 9, 015011.	4.4	5
78	First-principles approach to the electron transport and applications for devices based on carbon nanotubes and ultrathin oxides. Computer Physics Communications, 2007, 177, 30-33.	7.5	4
79	Diameter Dependence of Charge Transport across Carbon Nanotube?i>1/2Metal Contacts from First Principles. Journal of the Korean Physical Society, 2009, 55, 299-303.	0.7	3
80	An Optogeneticsâ€ Inspired Flexible van der Waals Optoelectronic Synapse and its Application to a Convolutional Neural Network (Adv. Mater. 40/2021). Advanced Materials, 2021, 33, 2170316.	21.0	3
81	Parallel Alignment of Methylammonium Cations in an Orthorhombic CH₃NH₃PbCl₃ Single Crystal Observed by Polarized Micro-Raman Scattering Spectroscopy. Chemistry of Materials, 2022, 34, 2972-2980.	6.7	3
82	Boron-Vacancy Pairing and Its Effect on the Electronic Properties of Carbon Nanotubes. ECS Solid State Letters, 2012, 1, M19-M23.	1.4	2
83	Carbon Fibers: Origin and Control of Polyacrylonitrile Alignments on Carbon Nanotubes and Graphene Nanoribbons (Adv. Funct. Mater. 15/2018). Advanced Functional Materials, 2018, 28, 1870099.	14.9	2
84	Carbon Nanotubes: Distinct Mechanisms of DNA Sensing Based on N-Doped Carbon Nanotubes with Enhanced Conductance and Chemical Selectivity (Small 4/2014). Small, 2014, 10, 622-622.	10.0	1
85	Theoretical Analysis and Experimental Optimization of Graphene/TMD Heterojunction Barristors. ECS Transactions, 2016, 75, 43-48.	0.5	1
86	Perovskite Nanowires: Semimetallicity and Negative Differential Resistance from Hybrid Halide Perovskite Nanowires (Adv. Funct. Mater. 13/2019). Advanced Functional Materials, 2019, 29, 1970084.	14.9	1
87	Density-functional study of the hydrogen-bonded water cluster H[sub 5]O[sub 2][sup +]. AIP Conference Proceedings, 2000, , .	0.4	0
88	First-principles study of charge transport across alkene thiolate self-assembled monolayers. , 2006, , .		0
89	Photocatalysts: Energy States of a Core-Shell Metal Oxide Photocatalyst Enabling Visible Light Absorption and Utilization in Solar-to-Fuel Conversion of Carbon Dioxide (Adv. Energy Mater. 14/2016). Advanced Energy Materials, 2016, 6, .	19.5	0
90	Data for quantum phonon transport in strained carbon atomic chains bridging graphene and graphene nanoribbon electrodes. Data in Brief, 2018, 21, 2421-2429.	1.0	0

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91	Performance Degradation in Graphene/ZnO Barristors Due to Graphene Edge Contact. ACS Applied Materials & Interfaces, 2020, 12, 28768-28774.	8.0	0
92	2D Electrides: MXene Phase with C ₃ Structure Unit: A Family of 2D Electrides (Adv. Funct. Mater.)	14.9	0
93	First-principles Electronic Structure Calculations for Renewable Energy Research: Examples and Prospects. Physics and High Technology, 2012, 21, 9.	0.1	0
94	First-Principles Nonequilibrium Quantum Transport Calculations and Their Applications to Next-Generation Nanoelectronic Devices. Physics and High Technology, 2017, 26, 8-14.	0.1	0