# Yong-Hoon Kim

List of Publications by Year
in descending order



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|---|---|---|---|
| 94 papers | 2,845 citations | 186209 28 h-index | 182361 51 g-index |
| 97 all docs | 97 docs citations | 97 times ranked | 3787 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Brainâ€Inspired Photonic Neuromorphic Devices using Photodynamic Amorphous Oxide Semiconductors and their Persistent Photoconductivity. Advanced Materials, 2017, 29, 1700951. | 11.1 | 346 |
| 2 | Structures and Properties of Self-Assembled Monolayers of Bistable [2]Rotaxanes on Au (111) Surfaces from Molecular Dynamics Simulations Validated with Experiment. Journal of the American Chemical Society, 2005, 127, 1563-1575. | 6.6 | 202 |
| 3 | Two-dimensional limit of exchange-correlation energy functional approximations. Physical Review B, 2000, 61, 5202-5211. | 1.1 | 129 |
| 4 | Excitonic Optical Spectrum of Semiconductors Obtained by Time-Dependent Density-Functional Theory with the Exact-Exchange Kernel. Physical Review Letters, 2002, 89, 096402. | 2.9 | 111 |
| 5 | Molecular Dynamics Simulation of Amphiphilic Bistable [2]Rotaxane Langmuir Monolayers at the Air/Water Interface. Journal of the American Chemical Society, 2005, 127, 14804-14816. | 6.6 | 102 |
| 6 | Modulation of the Electronic Properties of MXene (Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>) via Surface-Covalent Functionalization with Diazonium. ACS Nano, 2021, 15, 1388-1396. | 7.3 | 100 |
| 7 | Extremely Large Gate Modulation in Vertical Graphene/WSe<sub>2</sub> Heterojunction Barristor Based on a Novel Transport Mechanism. Advanced Materials, 2016, 28, 5293-5299. | 11.1 | 92 |
| 8 | Edge-selenated graphene nanoplatelets as durable metal-free catalysts for iodine reduction reaction in dye-sensitized solar cells. Science Advances, 2016, 2, e1501459. | 4.7 | 88 |
| 9 | Insight into the Microenvironments of the Metalâ€“Ionic Liquid Interface during Electrochemical CO<sub>2</sub> Reduction. ACS Catalysis, 2018, 8, 2420-2427. | 5.5 | 77 |
| 10 | Density Functional Theory Studies of the [2]Rotaxane Component of the Stoddartâˆ’Heath Molecular Switch. Journal of the American Chemical Society, 2004, 126, 12636-12645. | 6.6 | 74 |
| 11 | First-Principles Study of the Switching Mechanism of [2]Catenane Molecular Electronic Devices. Physical Review Letters, 2005, 94, 156801. | 2.9 | 72 |
| 12 | Exact Kohn-Sham exchange kernel for insulators and its long-wavelength behavior. Physical Review B, 2002, 66, . | 1.1 | 71 |
| 13 | An Optogeneticsâ€Inspired Flexible van der Waals Optoelectronic Synapse and its Application to a Convolutional Neural Network. Advanced Materials, 2021, 33, e2102980. | 11.1 | 65 |
| 14 | Ab initio study of the effect of water adsorption on the carbon nanotube field-effect transistor. Applied Physics Letters, 2006, 89, 243110. | 1.5 | 63 |
| 15 | Coherent Lattice Vibrations in Mono- and Few-Layer WSe<sub>2</sub>. ACS Nano, 2016, 10, 5560-5566. | 7.3 | 62 |
| 16 | First-principles approach to the charge-transport characteristics of monolayer molecular-electronics devices: Application to hexanedithiolate devices. Physical Review B, 2006, 73, . | 1.1 | 60 |
| 17 | Ultrafast Discharge/Charge Rate and Robust Cycle Life for Highâ€Performance Energy Storage Using Ultrafine Nanocrystals on the Binderâ€Free Porous Graphene Foam. Advanced Functional Materials, 2016, 26, 5139-5148. | 7.8 | 53 |
| 18 | Recent progress in atomistic simulation of electrical current DNA sequencing. Biosensors and Bioelectronics, 2015, 69, 186-198. | 5.3 | 48 |

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|---|---|---|---|
| 19 | HfO<sub>2</sub>/HfS<sub>2</sub> hybrid heterostructure fabricated via controllable chemical conversion of two-dimensional HfS<sub>2</sub>. Nanoscale, 2018, 10, 18758-18766. | 2.8 | 48 |
| 20 | Density-functional study of small molecules within the Krieger-Li-Iafrate approximation. Physical Review A, 1999, 60, 3633-3640. | 1.0 | 46 |
| 21 | Atomic-scale view of stability and degradation of single-crystal MAPbBr<sub>3</sub> surfaces. Journal of Materials Chemistry A, 2019, 7, 20760-20766. | 5.2 | 46 |
| 22 | Conformations and charge transport characteristics of biphenyldithiol self-assembled-monolayer molecular electronic devices: A multiscale computational study. Journal of Chemical Physics, 2005, 122, 244703. | 1.2 | 44 |
| 23 | Origins of genuine Ohmic van der Waals contact between indium and MoS2. Npj 2D Materials and Applications, 2021, 5, . | 3.9 | 43 |
| 24 | Shell-filling effects and Coulomb degeneracy in planar quantum-dot structures. Physical Review B, 1997, 56, 15752-15759. | 1.1 | 36 |
| 25 | Direct and defect-assisted electron tunneling through ultrathin<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> from first principles. Physical Review B, 2008, 77, . | 1.1 | 35 |
| 26 | Electronic and magnetic properties of carbide MXenesâ€”the role of electron correlations. Materials Today Advances, 2021, 9, 100118. | 2.5 | 35 |
| 27 | One-way multigrid method in electronic-structure calculations. Physical Review B, 2000, 61, 4397-4400. | 1.1 | 32 |
| 28 | Atomistic mechanisms of codoping-induced p- to n-type conversion in nitrogen-doped graphene. Nanoscale, 2014, 6, 14911-14918. | 2.8 | 30 |
| 29 | Stretching-Induced Conductance Variations as Fingerprints of Contact Configurations in Single-Molecule Junctions. Journal of the American Chemical Society, 2017, 139, 8286-8294. | 6.6 | 29 |
| 30 | Epitaxially Selfâ€Assembled Alkane Layers for Graphene Electronics. Advanced Materials, 2017, 29, 1603925. | 11.1 | 24 |
| 31 | Efficiency of Ï€âˆ’Ï€ Tunneling in [2]Rotaxane Molecular Electronic Switches. Journal of Physical Chemistry C, 2007, 111, 4831-4837. | 1.5 | 23 |
| 32 | Quantum interference in DNA bases probed by graphene nanoribbons. Applied Physics Letters, 2013, 103, . | 1.5 | 22 |
| 33 | Solution-processed oxide semiconductor-based artificial optoelectronic synapse array for spatiotemporal synaptic integration. Journal of Alloys and Compounds, 2021, 857, 158027. | 2.8 | 22 |
| 34 | Density Functional Theory Study of the Geometry, Energetics, and Reconstruction Process of Si(111) Surfaces. Langmuir, 2005, 21, 12404-12414. | 1.6 | 21 |
| 35 | Origin and Control of Polyacrylonitrile Alignments on Carbon Nanotubes and Graphene Nanoribbons. Advanced Functional Materials, 2018, 28, 1706970. | 7.8 | 18 |
| 36 | Raman Scattering Studies of the Structural Phase Transitions in Single-Crystalline CH<sub>3</sub>NH<sub>3</sub>PbCl<sub>3</sub>. Journal of Physical Chemistry Letters, 2020, 11, 3773-3781. | 2.1 | 18 |

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| 37 | Energy States of a Coreâ€Shell Metal Oxide Photocatalyst Enabling Visible Light Absorption and Utilization in Solarâ€toâ€Fuel Conversion of Carbon Dioxide. Advanced Energy Materials, 2016, 6, 1600583. | 10.2 | 17 |
| 38 | Electrical transport properties of nanoscale devices based on carbon nanotubes. Current Applied Physics, 2009, 9, S7-S11. | 1.1 | 16 |
| 39 | Conformational and conductance fluctuations in a single-molecule junction: Multiscale computational study. Physical Review B, 2010, 82, . | 1.1 | 16 |
| 40 | Capacitive energies of quantum dots with hydrogenic impurity. Physical Review B, 1999, 60, 13720-13726. | 1.1 | 15 |
| 41 | Semimetallicity and Negative Differential Resistance from Hybrid Halide Perovskite Nanowires. Advanced Functional Materials, 2019, 29, 1807620. | 7.8 | 15 |
| 42 | Surface Termination-Dependent Nanotribological Properties of Single-Crystal MAPbBr<sub>3</sub> Surfaces. Journal of Physical Chemistry C, 2020, 124, 1484-1491. | 1.5 | 15 |
| 43 | Strain-Induced Metallization and Defect Suppression at Zipper-like Interdigitated Atomically Thin Interfaces Enabling High-Efficiency Halide Perovskite Solar Cells. ACS Nano, 2021, 15, 1805-1816. | 7.3 | 15 |
| 44 | Conductance recovery and spin polarization in boron and nitrogen co-doped graphene nanoribbons. Carbon, 2015, 81, 339-346. | 5.4 | 14 |
| 45 | Quasi-Fermi level splitting in nanoscale junctions from ab initio. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 10142-10148. | 3.3 | 14 |
| 46 | Anomalous length scaling of carbon nanotube-metal contact resistance: An ab initio study. Applied Physics Letters, 2012, 100, 213113. | 1.5 | 13 |
| 47 | A facile synthesis of multi metal-doped rectangular ZnO nanocrystals using a nanocrystalline metalâ€“organic framework template. Nanoscale, 2014, 6, 10995-11001. | 2.8 | 13 |
| 48 | Carbon nanobuds based on carbon nanotube caps: a first-principles study. Nanoscale, 2016, 8, 2343-2349. | 2.8 | 13 |
| 49 | Highly luminescent blue-emitting CdZnS/ZnS nanorods having electric-field-induced fluorescence switching properties. Journal of Materials Chemistry C, 2017, 5, 2098-2106. | 2.7 | 13 |
| 50 | MXene Phase with C<sub>3</sub> Structure Unit: A Family of 2D Electrides. Advanced Functional Materials, 2021, 31, 2100009. | 7.8 | 13 |
| 51 | All-Inkjet-Printed Vertical Heterostructure for Wafer-Scale Electronics. ACS Nano, 2019, 13, 8213-8221. | 7.3 | 12 |
| 52 | Atomistics of Asymmetric Lateral Growth of Colloidal Zincblende CdSe Nanoplatelets. Chemistry of Materials, 2021, 33, 4813-4820. | 3.2 | 12 |
| 53 | Electronic structure of ellipsoidally deformed quantum dots. Journal of Physics Condensed Matter, 2001, 13, 1987-1993. | 0.7 | 11 |
| 54 | First-principles study of the electrical conductance of telescopically aligned carbon nanotubes. Physical Review B, 2007, 76, . | 1.1 | 11 |

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| 55 | Charge Transport through Polyene Self-Assembled Monolayers from Multiscale Computer Simulations. Journal of Physical Chemistry B, 2008, 112, 14888-14897. | 1.2 | 11 |
| 56 | Distinct Mechanisms of DNA Sensing Based on Nâ€Doped Carbon Nanotubes with Enhanced Conductance and Chemical Selectivity. Small, 2014, 10, 774-781. | 5.2 | 11 |
| 57 | Design and optimization of cobalt-encapsulating vertical graphene nano-hills for hydrogen evolution reaction. Journal of Materials Chemistry A, 2019, 7, 17046-17052. | 5.2 | 11 |
| 58 | Atomistic mechanisms of seeding promoter-controlled growth of molybdenum disulphide. 2D Materials, 2020, 7, 015013. | 2.0 | 11 |
| 59 | Possible performance improvement in [2]catenane molecular electronic switches. Applied Physics Letters, 2006, 88, 163112. | 1.5 | 9 |
| 60 | Intrinsically low-resistance carbon nanotube-metal contacts mediated by topological defects. MRS Communications, 2012, 2, 91-96. | 0.8 | 9 |
| 61 | Prediction of ultra-high ON/OFF ratio nanoelectromechanical switching from covalently-bound C60 chains. Carbon, 2014, 67, 48-57. | 5.4 | 9 |
| 62 | Nitrogen Doping of Carbon Nanoelectrodes for Enhanced Control of DNA Translocation Dynamics. ACS Applied Materials & Interfaces, 2018, 10, 18227-18236. | 4.0 | 9 |
| 63 | Odd-even phonon transport effects in strained carbon atomic chains bridging graphene nanoribbon electrodes. Carbon, 2019, 142, 107-114. | 5.4 | 9 |
| 64 | First-principles-derived effective mass approximation for the improved description of quantum nanostructures. JPhys Materials, 2020, 3, 034012. | 1.8 | 9 |
| 65 | Toward Numerically Accurate First-Principles Calculations of Nano-Device Charge Transport Characteristics: The Case of Alkane Single-Molecule Junctions. Journal of the Korean Physical Society, 2008, 52, 1181-1186. | 0.3 | 9 |
| 66 | Electrical and Mechanical Switching in a Realistic [2]Rotaxane Device Model. Journal of Nanoscience and Nanotechnology, 2008, 8, 4593-4597. | 0.9 | 8 |
| 67 | Multiâ€Space Excitation as an Alternative to the Landauer Picture for Nonequilibrium Quantum Transport. Advanced Science, 2020, 7, 2001038. | 5.6 | 8 |
| 68 | Valley depolarization in monolayer transition-metal dichalcogenides with zone-corner acoustic phonons. Nanoscale, 2020, 12, 22487-22494. | 2.8 | 8 |
| 69 | Emergence of multiple negative differential transconductance from a WSe2 double lateral homojunction platform. Applied Surface Science, 2022, 581, 152396. | 3.1 | 8 |
| 70 | Gate- versus defect-induced voltage drop and negative differential resistance in vertical graphene heterostructures. Npj Computational Materials, 2022, 8, . | 3.5 | 8 |
| 71 | Object-oriented construction of a multigrid electronic-structure code with Fortran 90. Computer Physics Communications, 2000, 131, 10-25. | 3.0 | 6 |
| 72 | Optical excitations of Si by time-dependent density functional theory based on exact-exchange Kohn-Sham band structure. International Journal of Quantum Chemistry, 2003, 91, 257-262. | 1.0 | 6 |

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| 73 | Metal-Independent Coherent Electron Tunneling through Polymerized Fullerene Chains. Journal of Physical Chemistry C, 2008, 112, 7029-7035. | 1.5 | 6 |
| 74 | Anomalous transport properties in boron and phosphorus co-doped armchair graphene nanoribbons. Nanotechnology, 2016, 27, 47LT01. | 1.3 | 6 |
| 75 | Zero power infrared sensing in 2D/3D-assembled heterogeneous graphene/In/InSe/Au. Nanoscale, 2022, 14, 3004-3012. | 2.8 | 6 |
| 76 | Quantum hybridization negative differential resistance from non-toxic halide perovskite nanowire heterojunctions and its strain control. Nano Convergence, 2022, 9, . | 6.3 | 6 |
| 77 | Shear-strain-mediated photoluminescence manipulation in two-dimensional transition metal dichalcogenides. 2D Materials, 2022, 9, 015011. | 2.0 | 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. | 3.0 | 4 |
| 79 | Diameter Dependence of Charge Transport across Carbon Nanotube?ï¿½Metal Contacts from First Principles. Journal of the Korean Physical Society, 2009, 55, 299-303. | 0.3 | 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. | 11.1 | 3 |
| 81 | Parallel Alignment of Methylammonium Cations in an Orthorhombic CH<sub>3</sub>NH<sub>3</sub>PbCl<sub>3</sub> Single Crystal Observed by Polarized Micro-Raman Scattering Spectroscopy. Chemistry of Materials, 2022, 34, 2972-2980. | 3.2 | 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. | 7.8 | 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. | 5.2 | 1 |
| 85 | Theoretical Analysis and Experimental Optimization of Graphene/TMD Heterojunction Barristors. ECS Transactions, 2016, 75, 43-48. | 0.3 | 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. | 7.8 | 1 |
| 87 | Density-functional study of the hydrogen-bonded water cluster H[sub 5]O[sub 2][sup +]. AIP Conference Proceedings, 2000, , . | 0.3 | 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, . | 10.2 | 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. | 0.5 | 0 |

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| 91 | Performance Degradation in Grapheneâ€“ZnO Barristors Due to Graphene Edge Contact. ACS Applied Materials & Interfaces, 2020, 12, 28768-28774. | 4.0 | 0 |
| 92 | 2D Electrides: MXene Phase with C<sub>3</sub> Structure Unit: A Family of 2D Electrides (Adv. Funct.) Tj ETQq0 0 0 rgBT /Overlock 10 | 7.8 | 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 |