# Abhishek K Singh

List of Publications by Year
in descending order

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Version: 2024-02-01

| 172 | 8,946 | 43973 | 48 | 48187 | 88 |
|---|---|---|---|---|---|
| papers | citations | | h-index | | g-index |

| 175 | 175 | 175 | 11562 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Pressure-induced semiconducting to metallic transition in multilayered molybdenum disulphide. Nature Communications, 2014, 5, 3731. | 5.8 | 495 |
| 2 | Sources of Electrical Conductivity in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>SnO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2008, 101, 055502. | 2.9 | 352 |
| 3 | Pressure-Dependent Optical and Vibrational Properties of Monolayer Molybdenum Disulfide. Nano Letters, 2015, 15, 346-353. | 4.5 | 284 |
| 4 | Semiconductor-metal transition in semiconducting bilayer sheets of transition-metal dichalcogenides. Physical Review B, 2012, 86, . | 1.1 | 259 |
| 5 | Recent advances in MXenes: From fundamentals to applications. Current Opinion in Solid State and Materials Science, 2019, 23, 164-178. | 5.6 | 247 |
| 6 | High-Entropy Alloys as Catalysts for the CO<sub>2</sub> and CO Reduction Reactions: Experimental Realization. ACS Catalysis, 2020, 10, 3658-3663. | 5.5 | 244 |
| 7 | Electronics and Magnetism of Patterned Graphene Nanoroads. Nano Letters, 2009, 9, 1540-1543. | 4.5 | 235 |
| 8 | Machine-Learning-Assisted Accurate Band Gap Predictions of Functionalized MXene. Chemistry of Materials, 2018, 30, 4031-4038. | 3.2 | 235 |
| 9 | C2N/WS2 van der Waals type-II heterostructure as a promising water splitting photocatalyst. Journal of Catalysis, 2018, 359, 143-150. | 3.1 | 229 |
| 10 | Mechanistic Insight into the Chemical Exfoliation and Functionalization of Ti<sub>3</sub>C<sub>2</sub> MXene. ACS Applied Materials & Interfaces, 2016, 8, 24256-24264. | 4.0 | 221 |
| 11 | Ferroelectricity, Antiferroelectricity, and Ultrathin 2D Electron/Hole Gas in Multifunctional Monolayer MXene. Nano Letters, 2017, 17, 3290-3296. | 4.5 | 184 |
| 12 | Magnetism in Transition-Metal-Doped Silicon Nanotubes. Physical Review Letters, 2003, 91, 146802. | 2.9 | 175 |
| 13 | Emerging 2D metal oxides and their applications. Materials Today, 2021, 45, 142-168. | 8.3 | 164 |
| 14 | Clustering of Sc on SWNT and Reduction of Hydrogen Uptake:â€‰ Ab-Initio All-Electron Calculations. Journal of Physical Chemistry C, 2007, 111, 17977-17980. | 1.5 | 159 |
| 15 | Atomically thin gallium layers from solid-melt exfoliation. Science Advances, 2018, 4, e1701373. | 4.7 | 157 |
| 16 | A new class of high strength high temperature Cobalt based Î³â€“Î³â€² Coâ€“Moâ€“Al alloys stabilized with Ta addition. Acta Materialia, 2015, 97, 29-40. | 3.8 | 151 |
| 17 | Hydrogen Evolution Reaction Activity of Grapheneâ€“MoS<sub>2</sub> van der Waals Heterostructures. ACS Energy Letters, 2017, 2, 1355-1361. | 8.8 | 141 |
| 18 | Probing Properties of Boron Î±-Tubes by Ab Initio Calculations. Nano Letters, 2008, 8, 1314-1317. | 4.5 | 140 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Quantum Dots and Nanoroads of Graphene Embedded in Hexagonal Boron Nitride. Journal of Physical Chemistry C, 2011, 115, 9889-9893. | 1.5 | 135 |
| 20 | H-Spillover through the Catalyst Saturation: An Ab Initio Thermodynamics Study. ACS Nano, 2009, 3, 1657-1662. | 7.3 | 127 |
| 21 | Magnetism in two-dimensional materials beyond graphene. Materials Today, 2019, 27, 107-122. | 8.3 | 127 |
| 22 | Fluorinated h-BN as a magnetic semiconductor. Science Advances, 2017, 3, e1700842. | 4.7 | 121 |
| 23 | Patterning nanoroads and quantum dots on fluorinated graphene. Nano Research, 2011, 4, 143-152. | 5.8 | 120 |
| 24 | Vacancy Clusters in Graphane as Quantum Dots. ACS Nano, 2010, 4, 3510-3514. | 7.3 | 119 |
| 25 | Boron doped defective graphene as a potential anode material for Li-ion batteries. Physical Chemistry Chemical Physics, 2014, 16, 16502. | 1.3 | 111 |
| 26 | Effect of strain on electronic and thermoelectric properties of few layers to bulk MoS<sub>2</sub>. Nanotechnology, 2014, 25, 465701. | 1.3 | 101 |
| 27 | Calcium-Decorated Carbyne Networks as Hydrogen Storage Media. Nano Letters, 2011, 11, 2660-2665. | 4.5 | 98 |
| 28 | Cluster Assembled Metal Encapsulated Thin Nanotubes of Silicon. Nano Letters, 2002, 2, 1243-1248. | 4.5 | 96 |
| 29 | Smallest Magic Caged Clusters of Si, Ge, Sn, and Pb by Encapsulation of Transition Metal Atom. Nano Letters, 2004, 4, 677-681. | 4.5 | 89 |
| 30 | Li diffusion through doped and defected graphene. Physical Chemistry Chemical Physics, 2013, 15, 15128. | 1.3 | 86 |
| 31 | pentahexoctite: A new two-dimensional allotrope of carbon. Scientific Reports, 2014, 4, 7164. | 1.6 | 85 |
| 32 | Semiconductor to metal transition in bilayer phosphorene under normal compressive strain. Nanotechnology, 2015, 26, 075701. | 1.3 | 83 |
| 33 | An amine functionalized zirconium metalâ€“organic framework as an effective chemiresistive sensor for acidic gases. Chemical Communications, 2019, 55, 349-352. | 2.2 | 83 |
| 34 | A Non-van der Waals Two-Dimensional Material from Natural Titanium Mineral Ore Ilmenite. Chemistry of Materials, 2018, 30, 5923-5931. | 3.2 | 82 |
| 35 | Effects of Morphology and Doping on the Electronic and Structural Properties of Hydrogenated Silicon Nanowires. Nano Letters, 2006, 6, 920-925. | 4.5 | 78 |
| 36 | Thermal Conductivity Enhancement in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>MoS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> under Extreme Strain. Physical Review Letters, 2019, 122, 155901. | 2.9 | 75 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | High temperature thermoelectric properties of Zr and Hf based transition metal dichalcogenides: A first principles study. Journal of Chemical Physics, 2015, 143, 234704. | 1.2 | 72 |
| 38 | Origin of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>n</mml:mi></mml:math> -type conductivity of monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mm Physical Review B, 2019, 99, . | 1.1 | 72 |
| 39 | The ultimate diamond slab: GraphAne versus graphEne. Diamond and Related Materials, 2010, 19, 368-373. | 1.8 | 71 |
| 40 | Origin of Ultralow Thermal Conductivity in n-Type Cubic Bulk AgBiS<sub>2</sub>: Soft Ag Vibrations and Local Structural Distortion Induced by the Bi 6s<sup>2</sup> Lone Pair. Chemistry of Materials, 2019, 31, 2106-2113. | 3.2 | 70 |
| 41 | Hydrogen interactions with acceptor impurities in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SnO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms First-principles calculations. Physical Review B, 2009, 79, . | 1.1 | 63 |
| 42 | Coupling the High-Throughput Property Map to Machine Learning for Predicting Lattice Thermal Conductivity. Chemistry of Materials, 2019, 31, 5145-5151. | 3.2 | 63 |
| 43 | Effect of Cr addition on Î³â€“Î³â€² cobalt-based Coâ€“Moâ€“Alâ€“Ta class of superalloys: a combined experimental and computational study. Journal of Materials Science, 2017, 52, 11036-11047. | 1.7 | 61 |
| 44 | The Boron Buckyball and Its Precursors: An Electronic Structure Study. Journal of Physical Chemistry A, 2008, 112, 13679-13683. | 1.1 | 57 |
| 45 | Noble-Metal-Free Heterojunction Photocatalyst for Selective CO<sub>2</sub> Reduction to Methane upon Induced Strain Relaxation. ACS Catalysis, 2022, 12, 687-697. | 5.5 | 56 |
| 46 | Metallacarboranes: Toward Promising Hydrogen Storage Metal Organic Frameworks. Journal of the American Chemical Society, 2010, 132, 14126-14129. | 6.6 | 55 |
| 47 | Stabilizing the silicon fullereneSi20by thorium encapsulation. Physical Review B, 2005, 71, . | 1.1 | 54 |
| 48 | Hydrogen Storage Capacity of Carbon-Foams: Grand Canonical Monte Carlo Simulations. Journal of Physical Chemistry C, 2011, 115, 2476-2482. | 1.5 | 51 |
| 49 | Metal encapsulated nanotubes of silicon and germanium. Journal of Materials Chemistry, 2004, 14, 555. | 6.7 | 49 |
| 50 | Strain-induced indirect-to-direct band-gap transition in bulk <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SnS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:msub></mm Physical Review B, 2017, 95, . | 1.1 | 49 |
| 51 | Charged and magnetic fullerenes of silicon by metal encapsulation: Predictions fromab initiocalculations. Physical Review B, 2006, 74, . | 1.1 | 47 |
| 52 | Isolation of pristine MXene from Nb<sub>4</sub>AlC<sub>3</sub> MAX phase: a first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 11073-11080. | 1.3 | 47 |
| 53 | Electrooxidation of Hydrazine Utilizing High-Entropy Alloys: Assisting the Oxygen Evolution Reaction at the Thermodynamic Voltage. ACS Catalysis, 2021, 11, 14000-14007. | 5.5 | 47 |
| 54 | Mechanical and electronic properties of pristine and Ni-doped Si, Ge, and Sn sheets. Physical Chemistry Chemical Physics, 2014, 16, 1667-1671. | 1.3 | 46 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | Pressureâ€Induced Charge Transfer Doping of Monolayer Graphene/MoS<sub>2</sub> Heterostructure. Small, 2016, 12, 4063-4069. | 5.2 | 45 |
| 56 | Atomistic Origin of Phase Stability in Oxygen-Functionalized MXene: A Comparative Study. Journal of Physical Chemistry C, 2017, 121, 18947-18953. | 1.5 | 44 |
| 57 | Accelerated Data-Driven Accurate Positioning of the Band Edges of MXenes. Journal of Physical Chemistry Letters, 2019, 10, 780-785. | 2.1 | 43 |
| 58 | Nanostructured Tungsten Oxysulfide as an Efficient Electrocatalyst for Hydrogen Evolution Reaction. ACS Catalysis, 2020, 10, 6753-6762. | 5.5 | 43 |
| 59 | Multi-component (Agâ€“Auâ€“Cuâ€“Pdâ€“Pt) alloy nanoparticle-decorated p-type 2D-molybdenum disulfide (MoS<sub>2</sub>) for enhanced hydrogen sensing. Nanoscale, 2020, 12, 11830-11841. | 2.8 | 42 |
| 60 | High performance Ni-substituted Mnâ€“Zn ferrites processed by soft chemical technique. Journal of Magnetism and Magnetic Materials, 2004, 281, 276-280. | 1.0 | 41 |
| 61 | Pristine Semiconducting [110] Silicon Nanowires. Nano Letters, 2005, 5, 2302-2305. | 4.5 | 40 |
| 62 | Accelerated prediction of Vickers hardness of Co- and Ni-based superalloys from microstructure and composition using advanced image processing techniques and machine learning. Acta Materialia, 2020, 196, 295-303. | 3.8 | 40 |
| 63 | Chemical hardness-driven interpretable machine learning approach for rapid search of photocatalysts. Npj Computational Materials, 2021, 7, . | 3.5 | 40 |
| 64 | Inner Sphere Electron Transfer Promotion on Homogeneously Dispersed Fe-N<sub>x</sub> Centers for Energy-Efficient Oxygen Reduction Reaction. ACS Applied Materials & Interfaces, 2020, 12, 36026-36039. | 4.0 | 39 |
| 65 | Formic acid and methanol electro-oxidation and counter hydrogen production using nano high entropy catalyst. Materials Today Energy, 2020, 16, 100393. | 2.5 | 38 |
| 66 | Stackingâ€Orderâ€Driven Optical Properties and Carrier Dynamics in ReS<sub>2</sub>. Advanced Materials, 2020, 32, e1908311. | 11.1 | 38 |
| 67 | Insulating State and Breakdown of Fermi Liquid Description in Molecular-Scale Single-Crystalline Wires of Gold. ACS Nano, 2011, 5, 8398-8403. | 7.3 | 36 |
| 68 | Wrinkling of Atomic Planes in Ultrathin Au Nanowires. Nano Letters, 2014, 14, 4859-4866. | 4.5 | 35 |
| 69 | Diffusive nature of thermal transport in stanene. Physical Chemistry Chemical Physics, 2016, 18, 14257-14263. | 1.3 | 34 |
| 70 | High Thermoelectric Performance in n-Doped Silicon-Based Chalcogenide Si<sub>2</sub>Te<sub>3</sub>. Chemistry of Materials, 2017, 29, 3723-3730. | 3.2 | 34 |
| 71 | Insights into nucleation, growth and phase selection of WO<sub>3</sub>: morphology control and electrochromic properties. Journal of Materials Chemistry C, 2017, 5, 7307-7316. | 2.7 | 34 |
| 72 | First principles calculations of H-storage in sorption materials. Journal of Materials Science, 2012, 47, 7356-7366. | 1.7 | 33 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | High thermopower and ultra low thermal conductivity in Cd-based Zintl phase compounds. Physical Chemistry Chemical Physics, 2015, 17, 16917-16926. | 1.3 | 33 |
| 74 | Morphology controlled synthesis of low bandgap SnSe<sub>2</sub> with high photodetectivity. Nanoscale, 2019, 11, 870-877. | 2.8 | 31 |
| 75 | Development of Vickers hardness prediction models via microstructural analysis and machine learning. Journal of Materials Science, 2020, 55, 15845-15856. | 1.7 | 30 |
| 76 | Thorium Encapsulated Caged Clusters of Germanium:Â Th@Gen,n= 16, 18, and 20. Journal of Physical Chemistry B, 2005, 109, 15187-15189. | 1.2 | 29 |
| 77 | Monolayer BC<sub>2</sub>: an ultrahigh capacity anode material for Li ion batteries. Physical Chemistry Chemical Physics, 2017, 19, 24230-24239. | 1.3 | 29 |
| 78 | Towards band structure and band offset engineering of monolayer Mo <sub> (1â^' x ) </sub> W <sub> ( x ) </sub> S <sub>2</sub> via Strain. 2D Materials, 2018, 5, 015008. | 2.0 | 28 |
| 79 | Engineering Defect Transition-Levels through the van der Waals Heterostructure. Journal of Physical Chemistry C, 2018, 122, 24475-24480. | 1.5 | 27 |
| 80 | An Insight into the Phase Transformation of WS<sub>2</sub> upon Fluorination. Advanced Materials, 2018, 30, e1803366. | 11.1 | 26 |
| 81 | Strong Chemical Bond Hierarchy Leading to Exceptionally High Thermoelectric Figure of Merit in Oxychalcogenide AgBiTeO. ACS Applied Materials & Interfaces, 2020, 12, 8280-8287. | 4.0 | 26 |
| 82 | Ultralow Thermal Conductivity in Earth-Abundant Cu<sub>1.6</sub>Bi<sub>4.8</sub>S<sub>8</sub>: Anharmonic Rattling of Interstitial Cu. Chemistry of Materials, 2021, 33, 2993-3001. | 3.2 | 26 |
| 83 | Single crystalline ultrathin gold nanowires: Promising nanoscale interconnects. AIP Advances, 2013, 3, . | 0.6 | 25 |
| 84 | Metalâ€Free Dual Modal Contrast Agents Based on Fluorographene Quantum Dots. Particle and Particle Systems Characterization, 2017, 34, 1600221. | 1.2 | 25 |
| 85 | High Thermoelectric Figure of Merit via Tunable Valley Convergence Coupled Low Thermal Conductivity in AIIBIVC2VChalcopyrites. Journal of Physical Chemistry C, 2018, 122, 29150-29157. | 1.5 | 25 |
| 86 | Rattling-Induced Ultralow Thermal Conductivity Leading to Exceptional Thermoelectric Performance in AgIn<sub>5</sub>S<sub>8</sub>. ACS Applied Materials & Interfaces, 2019, 11, 33894-33900. | 4.0 | 25 |
| 87 | Strain-induced electronic phase transition and strong enhancement of thermopower of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">TiS</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 90, . | 1.1 | 24 |
| 88 | Suppression of Jahnâ€“Teller Distortions and Origin of Piezochromism and Thermochromism in Cuâ€“Cl Hybrid Perovskite. Inorganic Chemistry, 2016, 55, 6817-6824. | 1.9 | 24 |
| 89 | Structural and spectroscopic characterizations of a new near-UV-converting cyan-emitting RbBaScSi3O9:Eu2+ phosphor with robust thermal performance. Journal of Alloys and Compounds, 2017, 713, 138-147. | 2.8 | 24 |
| 90 | Thermoelectric properties of Î²-FeSi2. Journal of Applied Physics, 2013, 114, . | 1.1 | 23 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | Ferromagnetism and piezomagnetic behavior in Mn-doped germanium nanotubes. Physical Review B, 2004, 69, . | 1.1 | 22 |
| 92 | Low formation energy and kinetic barrier of Stoneâ€“Wales defect in infinite and finite silicene. Chemical Physics Letters, 2014, 592, 52-55. | 1.2 | 22 |
| 93 | Remarkable enhancement in hydrogen storage on free-standing Ti 3 B and BC 3 supported Ti 3 clusters. International Journal of Hydrogen Energy, 2015, 40, 1054-1061. | 3.8 | 22 |
| 94 | Lifshitz transition and modulation of electronic and transport properties of bilayer graphene by sliding and applied normal compressive strain. Carbon, 2016, 99, 432-438. | 5.4 | 22 |
| 95 | A Statistical Approach for the Rapid Prediction of Electron Relaxation Time Using Elemental Representatives. Chemistry of Materials, 2020, 32, 6507-6514. | 3.2 | 22 |
| 96 | Unraveling the role of bonding chemistry in connecting electronic and thermal transport by machine learning. Journal of Materials Chemistry A, 2020, 8, 8716-8721. | 5.2 | 21 |
| 97 | New insights into designing metallacarborane based room temperature hydrogen storage media. Journal of Chemical Physics, 2013, 139, 164319. | 1.2 | 20 |
| 98 | Pt-Poisoning-Free Efficient CO Oxidation on Pt<sub>3</sub>Co Supported on MgO(100): An Ab Initio Study. ACS Catalysis, 2015, 5, 1826-1832. | 5.5 | 20 |
| 99 | Rational Design of Single-Atom Catalysts for Enhanced Electrocatalytic Nitrogen Reduction Reaction. Journal of Physical Chemistry C, 2021, 125, 12585-12593. | 1.5 | 20 |
| 100 | Simultaneous enhancement of electrical conductivity and thermopower in Bi<sub>2</sub>S<sub>3</sub> under hydrostatic pressure. Journal of Materials Chemistry C, 2016, 4, 1979-1987. | 2.7 | 19 |
| 101 | Graphene Oxide Epoxy (GOâ€xy): GO as Epoxy Adhesive by Interfacial Reaction of Functionalities. Advanced Materials Interfaces, 2018, 5, 1700657. | 1.9 | 19 |
| 102 | Design of a very thin direct-band-gap semiconductor nanotube of germanium with metal encapsulation. Physical Review B, 2005, 71, . | 1.1 | 18 |
| 103 | Strain-induced chiral symmetry breaking leads to large Dirac cone splitting in graphene/graphane heterostructure. Physical Review B, 2016, 94, . | 1.1 | 18 |
| 104 | Pressureâ€Dependent Behavior of Defectâ€Modulated Band Structure in Boron Arsenide. Advanced Materials, 2020, 32, e2001942. | 11.1 | 18 |
| 105 | Accelerated Discovery of the Valley-Polarized Quantum Anomalous Hall Effect in MXenes. Chemistry of Materials, 2021, 33, 6311-6317. | 3.2 | 18 |
| 106 | Structure of the thinnest most stable semiconducting and insulating nanotubes ofSiOx(x=1,2). Physical Review B, 2005, 72, . | 1.1 | 17 |
| 107 | Semiconductor-like Sensitivity in Metallic Ultrathin Gold Nanowire-Based Sensors. Journal of Physical Chemistry C, 2014, 118, 18676-18682. | 1.5 | 17 |
| 108 | Graphene-oxide-supported ultrathin Au nanowires: efficient electrocatalysts for borohydride oxidation. Chemical Communications, 2015, 51, 16856-16859. | 2.2 | 17 |

| # | Article | IF | Citations |
|---|---|---|---|
| 109 | Simultaneous tunability of the electronic and phononic gaps in SnS <sub>2</sub> under normal compressive strain. 2D Materials, 2016, 3, 015009. | 2.0 | 16 |
| 110 | Electronic Structure Based Intuitive Design Principle of Singleâ€Atom Catalysts for Efficient Electrolytic Nitrogen Reduction. ChemCatChem, 2020, 12, 5456-5464. | 1.8 | 16 |
| 111 | Ultralow thermal conductivity and high thermoelectric figure of merit in mixed valence In<sub>5</sub>X<sub>5</sub>Br (X = S, and Se) compounds. Journal of Materials Chemistry A, 2020, 8, 13812-13819. | 5.2 | 16 |
| 112 | Nonlinear Optical Absorption of ReS<sub>2</sub> Driven by Stacking Order. ACS Photonics, 2021, 8, 405-411. | 3.2 | 16 |
| 113 | Formation of a Small Electron Polaron in Tantalum Oxynitride: Origin of Low Mobility. Journal of Physical Chemistry C, 2021, 125, 11548-11554. | 1.5 | 16 |
| 114 | Simultaneous Site Adsorption Shift and Efficient CO Oxidation Induced by V and Co in Pt Catalyst. Journal of Physical Chemistry C, 2017, 121, 12807-12816. | 1.5 | 15 |
| 115 | Growth of Molybdenum Carbideâ€“Graphene Hybrids from Molybdenum Disulfide Atomic Layer Template. Advanced Materials Interfaces, 2017, 4, 1600866. | 1.9 | 14 |
| 116 | Topologically nontrivial electronic states in CaSn3. Journal of Applied Physics, 2017, 121, . | 1.1 | 14 |
| 117 | Existence of Ti<sup>2+</sup> States on the Surface of Heavily Reduced SrTiO<sub>3</sub> Nanocubes. Chemistry of Materials, 2017, 29, 9887-9891. | 3.2 | 14 |
| 118 | Pressure-Induced Topological Phase Transitions in CdGeSb<sub>2</sub> and CdSnSb<sub>2</sub>. Journal of Physical Chemistry Letters, 2018, 9, 2202-2207. | 2.1 | 14 |
| 119 | Structural, vibrational, and electronic topological transitions of Bi1.5Sb0.5Te1.8Se1.2 under pressure. Journal of Applied Physics, 2018, 123, . | 1.1 | 14 |
| 120 | Mechanistic study on nitrogen-doped graphitic carbon-reinforced chromium nitride as a durable electrocatalyst for oxygen reduction. Journal of Materials Chemistry A, 2021, 9, 16575-16584. | 5.2 | 14 |
| 121 | Orientation Selection during Heterogeneous Nucleation: Implications for Heterogeneous Catalysis. Journal of Physical Chemistry C, 2017, 121, 10027-10037. | 1.5 | 13 |
| 122 | Origamiâ€Inspired 3D Interconnected Molybdenum Carbide Nanoflakes. Advanced Materials Interfaces, 2018, 5, 1701113. | 1.9 | 13 |
| 123 | Guided patchwork kriging to develop highly transferable thermal conductivity prediction models. JPhys Materials, 2020, 3, 024006. | 1.8 | 13 |
| 124 | Metal encapsulated nanotubes of germanium with metal dependent electronic properties. European Physical Journal D, 2005, 34, 295-298. | 0.6 | 11 |
| 125 | Structural and magnetic stabilities of cubic and orthorhombic phases of CeMnNi4. Applied Physics Letters, 2006, 89, 222502. | 1.5 | 11 |
| 126 | Electroreduction of Carbon Dioxide into Selective Hydrocarbons at Low Overpotential Using Isomorphic Atomic Substitution in Copper Oxide. ACS Sustainable Chemistry and Engineering, 2020, 8, 179-189. | 3.2 | 11 |

| # | Article | IF | Citations |
|---|---|---|---|
| 127 | Anisotropic Interlayer Exciton in GeSe/SnS van der Waals Heterostructure. Journal of Physical Chemistry Letters, 2021, 12, 1765-1771. | 2.1 | 11 |
| 128 | Electronic transport in patterned graphene nanoroads. Nanotechnology, 2013, 24, 495201. | 1.3 | 10 |
| 129 | Synergistic coreâ€“shell interactions enable ultra-low overpotentials for enhanced CO<sub>2</sub> electro-reduction activity. Journal of Materials Chemistry A, 2018, 6, 21120-21130. | 5.2 | 10 |
| 130 | Atypical behavior of intrinsic defects and promising dopants in two-dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>WS</mml:mi></mml:mrow><mml:mn>2</m Physical Review Materials, 2021, 5, . | 3.0 | 10 |
| 131 | Armchair or Zigzag? A tool for characterizing graphene edge. Computer Physics Communications, 2011, 182, 804-807. | 3.0 | 9 |
| 132 | Ultra-sensitive pressure dependence of bandgap of rutile-GeO2 revealed by many body perturbation theory. Journal of Chemical Physics, 2015, 143, 064703. | 1.2 | 9 |
| 133 | Manipulation of Optoelectronic Properties and Band Structure Engineering of Ultrathin Te Nanowires by Chemical Adsorption. ACS Applied Materials & Interfaces, 2017, 9, 19462-19469. | 4.0 | 9 |
| 134 | Effective sensing radius (ESR) and performance analysis of static and mobile sensor networks. Telecommunication Systems, 2018, 68, 115-127. | 1.6 | 9 |
| 135 | Interfacial Electron Transfer Strategy to Improve the Hydrogen Evolution Catalysis of CrP Heterostructure. Small, 2022, 18, e2106139. | 5.2 | 9 |
| 136 | Origin of enhanced thermoelectric properties of doped CrSi<sub>2</sub>. RSC Advances, 2014, 4, 3482-3486. | 1.7 | 8 |
| 137 | Interferroelectric transition as another manifestation of intrinsic size effect in ferroelectrics. Physical Review B, 2016, 94, . | 1.1 | 8 |
| 138 | Multiple triple-point fermions in Heusler compounds. Journal of Physics Condensed Matter, 2018, 30, 375702. | 0.7 | 8 |
| 139 | Growth of highly crystalline ultrathin two-dimensional selenene. 2D Materials, 2022, 9, 045004. | 2.0 | 8 |
| 140 | Improvement in Oxygen Evolution Performance of NiFe Layered Double Hydroxide Grown in the Presence of 1T-Rich MoS<sub>2</sub>. ACS Applied Materials & Interfaces, 2022, 14, 31951-31961. | 4.0 | 8 |
| 141 | Mechanism for the Compressive Strain Induced Oscillations in the Conductance of Carbon Nanotubes. Physical Review Letters, 2013, 110, 095504. | 2.9 | 7 |
| 142 | Interplay of Structural and Bonding Characters in Thermal Conductivity and Born-Effective Charge of Transition Metal Dichalcogenides. Journal of Physical Chemistry C, 2018, 122, 2521-2527. | 1.5 | 7 |
| 143 | Noninvasive Subsurface Electrical Probe for Encapsulated Layers in van der Waals Heterostructures. Physical Review Applied, 2019, 12, . | 1.5 | 7 |
| 144 | Enhancing hydrogen storage capacity of pyridine-based metal organic framework. International Journal of Hydrogen Energy, 2014, 39, 9293-9299. | 3.8 | 6 |

| # | Article | IF | Citations |
|---|---|---|---|
| 145 | Negative differential resistance in armchair silicene nanoribbons. Nanotechnology, 2017, 28, 275402. | 1.3 | 6 |
| 146 | Reflection and Transmission of P-Waves in an Intermediate Layer Lying Between Two Semi-infinite Media. Pure and Applied Geophysics, 2018, 175, 4305-4319. | 0.8 | 6 |
| 147 | Revealing carbon mediated luminescence centers with enhanced lifetime in porous alumina. Journal of Applied Physics, 2019, 126, 164904. | 1.1 | 6 |
| 148 | Feature Blending: An Approach toward Generalized Machine Learning Models for Property Prediction. ACS Physical Chemistry Au, 2022, 2, 16-22. | 1.9 | 6 |
| 149 | Vacancy mediated clipping of multi-layered graphene: A precursor for 1, 2 and 3D carbon structures. Carbon, 2015, 94, 67-72. | 5.4 | 5 |
| 150 | â€œCappingâ€•out oxygen interference: An approach to achieve efficient hydrogen storage via Kubas binding. International Journal of Hydrogen Energy, 2016, 41, 5979-5985. | 3.8 | 5 |
| 151 | Nonlinear Polarization and Low-Dissipation Ultrafast Optical Switching in Phosphorene. Journal of Physical Chemistry C, 2018, 122, 19146-19152. | 1.5 | 5 |
| 152 | Layer parity dependent Raman-active modes and crystal symmetry in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">ReS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2022, 105, . | 1.1 | 5 |
| 153 | Origin of layer-dependent electrical conductivity of transition metal dichalcogenides. Physical Review B, 2022, 105, . | 1.1 | 5 |
| 154 | The influence of insulating substrate on the electrical measurements of focused ion beam fabricated electrodes with nano-gap spacing. Nuclear Instruments & Methods in Physics Research B, 2010, 268, 3282-3286. | 0.6 | 4 |
| 155 | Effect of ambient on electrical transport properties of ultra-thin Au nanowires. Applied Physics Letters, 2016, 109, 253108. | 1.5 | 4 |
| 156 | Topological Phases in Hydrogenated Group 13 Monolayers. Journal of Physical Chemistry C, 2019, 123, 25985-25990. | 1.5 | 4 |
| 157 | Electroreduction of CO<sub>2</sub> with Tunable Selectivity on Auâ€“Pd Bimetallic Catalyst: A First Principle Study. ACS Applied Materials & Interfaces, 2022, 14, 11313-11321. | 4.0 | 4 |
| 158 | Quantum confinement effect on defect level of hydrogen doped rutile VO2 nanowires. Journal of Applied Physics, 2022, 131, . | 1.1 | 4 |
| 159 | Decoupled atomic contribution boosted high thermoelectric performance in mixed cation spinel oxides ACo2O4. Applied Physics Letters, 2022, 120, . | 1.5 | 4 |
| 160 | Pressure induced manifold enhancement of Li-kinetics in FCC fullerene. Physical Chemistry Chemical Physics, 2014, 16, 21688-21693. | 1.3 | 3 |
| 161 | Structureâ€Ðependent Electrical and Magnetic Properties of Iron Oxide Composites. Physica Status Solidi (A) Applications and Materials Science, 2019, 216, 1801004. | 0.8 | 3 |
| 162 | First Principles Study on Structural Stability of Belite. ACI Materials Journal, 2015, 112, . | 0.3 | 3 |

| # | Article | IF | Citations |
|---|---|---|---|
| 163 | Diffusion-enhanced preferential growth of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e570" altimg="si37.svg"><mml:mi>m</mml:mi></mml:math>-oriented GaN micro-domains on directly grown graphene with a large domain size on Ti/SiO2/Si(001). Materials Today Communications, 2022, 30, 103113. | 0.9 | 3 |
| 164 | THEORETICAL ADVANCES IN THE ELECTRONIC AND ATOMIC STRUCTURES OF SILICON NANOTUBES AND NANOWIRES. , 2008, , 217-257. | | 2 |
| 165 | Critical Sublattice Symmetry Breaking: A Universal Criterion for Dirac Cone Splitting. Journal of Physical Chemistry C, 2019, 123, 23082-23088. | 1.5 | 2 |
| 166 | Carrier Dynamics in Ultrathin Gold Nanowires: Role of Auger Processes. Plasmonics, 2020, 15, 1151-1158. | 1.8 | 2 |
| 167 | Effect of the Edge Type and Strain on the Structural, Electronic and Magnetic Properties of the BNRs. Journal of Nanoscience and Nanotechnology, 2012, 12, 1899-1902. | 0.9 | 1 |
| 168 | Accelerated Discovery of Thermoelectric Materials Using Machine Learning. Springer Series in Materials Science, 2021, , 133-152. | 0.4 | 1 |
| 169 | Metal Encapsulated Nanotubes of Silicon and Germanium. ChemInform, 2004, 35, no. | 0.1 | 0 |
| 170 | Thorium Encapsulated Caged Clusters of Germanium: Th@Gen, n = 16,18, and 20.. ChemInform, 2005, 36, no. | 0.1 | 0 |
| 171 | Strain-induced phenomena in layered materials. , 2015, , . | | 0 |
| 172 | Tuning Catalytic Activity in Ultrathin Bimetallic Nanowires via Surface Segregation: Some Insights. Journal of Physical Chemistry Letters, 2022, 13, 770-776. | 2.1 | 0 |