# Sanjeev K Gupta

List of Publications by Year
in descending order



| 226 | 3,368 | 136740 | 214527 |
|---|---|---|---|
| papers | citations | 32 h-index | 47 g-index |

| 228 | 228 | 228 | 4051 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Synthesis of exfoliated multilayer graphene and its putative interactions with SARS-CoV-2 virus investigated through computational studies. Journal of Biomolecular Structure and Dynamics, 2022, 40, 712-721. | 2.0 | 17 |
| 2 | Mobility driven thermoelectric and optical properties of two-dimensional halide-based hybrid perovskites: impact of organic cation rotation. Physical Chemistry Chemical Physics, 2022, 24, 8867-8880. | 1.3 | 7 |
| 3 | Strain-mediated ferromagnetism and low-field magnetic reversal in Co doped monolayer $$WS_2$$. Scientific Reports, 2022, 12, 2593. | 1.6 | 10 |
| 4 | Strain modulating electronic band gaps and SQ efficiencies of semiconductor 2D PdQ2 (Qâ€‰=â€‰S, Se) monolayer. Scientific Reports, 2022, 12, 2964. | 1.6 | 19 |
| 5 | Electronic bandstructure modulation of MoX2/ZnO(X:S,Se) heterostructure by applying external electric field. Surfaces and Interfaces, 2022, 29, 101817. | 1.5 | 8 |
| 6 | Capacity development of Pd doped Si2BN nanotube for hydrogen storage. International Journal of Hydrogen Energy, 2022, 47, 19132-19145. | 3.8 | 6 |
| 7 | Ab-initio study of formamidinium lead halide (FAPbX3, XÂ=ÂBr, Cl) perovskiteâ€™s monolayers. Materials Today: Proceedings, 2022, 67, 20-24. | 0.9 | 0 |
| 8 | Selective and sensitive toxic gas-sensing mechanism in a 2D Janus MoSSe monolayer. Physical Chemistry Chemical Physics, 2022, 24, 15292-15304. | 1.3 | 13 |
| 9 | Prominent Electrode Material for Na-, K-, and Mg-ion Batteries: 2D Î²-Sb Monolayer. Energy & Fuels, 2022, 36, 7087-7095. | 2.5 | 16 |
| 10 | Systematic investigation of electronic, mechanical and optical properties of UO2 at higher pressure: A DFT+U+SOC study. Solid State Sciences, 2022, 132, 106968. | 1.5 | 2 |
| 11 | Transition metal substituted MoS2/WS2 van der Waals heterostructure for realization of dilute magnetic semiconductors. Journal of Magnetism and Magnetic Materials, 2022, 560, 169567. | 1.0 | 6 |
| 12 | Structural, electronic and optical properties of hexagonal boron-nitride (h-BN) monolayer: An Ab-initio study. Materials Today: Proceedings, 2021, 47, 529-532. | 0.9 | 13 |
| 13 | An ab-initio study of blue phosphorene monolayer: Electronic, vibrational and optical properties. Materials Today: Proceedings, 2021, 47, 576-579. | 0.9 | 2 |
| 14 | Ultrathin Pd and Pt nanowires for potential applications as hydrogen economy. Materials Today Communications, 2021, 26, 101761. | 0.9 | 4 |
| 15 | Ultrahigh carrier mobility and light-harvesting performance of 2D penta-PdX2 monolayer. Journal of Materials Science, 2021, 56, 3846-3860. | 1.7 | 24 |
| 16 | Mechanism of formaldehyde and formic acid formation on (101)-TiO<sub>2</sub>@Cu<sub>4</sub> systems through CO<sub>2</sub> hydrogenation. Sustainable Energy and Fuels, 2021, 5, 564-574. | 2.5 | 4 |
| 17 | Strain dependent electronic transport of pristine Si and Ge nanowires. Computational Materials Science, 2021, 188, 110181. | 1.4 | 3 |
| 18 | ZnS/CdX (X = S, Se, Te) core/shell nanowires: an attempt at tuning the electronic bandgaps and SQ efficiencies. Journal of Materials Chemistry C, 2021, 9, 6605-6617. | 2.7 | 4 |

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| 19 | Hydrogenation and oxidation enhances the thermoelectric performance of Si<sub>2</sub>BN monolayer. New Journal of Chemistry, 2021, 45, 3892-3900. | 1.4 | 8 |
| 20 | Carbon nanotubes for rapid capturing of SARS-COV-2 virus: revealing a mechanistic aspect of binding based on computational studies. RSC Advances, 2021, 11, 5785-5800. | 1.7 | 15 |
| 21 | Effect of Charge Injection on the Conducting Filament of Valence Change Anatase TiO<sub>2</sub> Resistive Random Access Memory Device. Journal of Physical Chemistry Letters, 2021, 12, 1876-1884. | 2.1 | 20 |
| 22 | Exploring the transport and optoelectronic properties of silicon diselenide monolayer. Superlattices and Microstructures, 2021, 150, 106813. | 1.4 | 9 |
| 23 | Diffusion of oxygen in hypostoichiometric uranium dioxide nanocrystals. A molecular dynamics simulation. Chimica Techno Acta, 2021, 8, 20218107. | 0.3 | 1 |
| 24 | Salt-assisted growth of monolayer MoS2 for high-performance hysteresis-free field-effect transistor. Journal of Applied Physics, 2021, 129, . | 1.1 | 19 |
| 25 | Azahomofullerenes as New n-Type Acceptor Materials for Efficient and Stable Inverted Planar Perovskite Solar Cells. ACS Applied Materials & Interfaces, 2021, 13, 20296-20304. | 4.0 | 13 |
| 26 | Van der waals SiSe2 homo-bilayers for optoelectronics applications. Superlattices and Microstructures, 2021, 152, 106858. | 1.4 | 18 |
| 27 | Atomistic investigations of melting characterization in metallic nanostructures. Surface Science, 2021, 707, 121803. | 0.8 | 2 |
| 28 | Antimonene Allotropes Î±- and Î²-Phases as Promising Anchoring Materials for Lithiumâ€“Sulfur Batteries. Energy & Fuels, 2021, 35, 9001-9009. | 2.5 | 15 |
| 29 | First-Principles Study of Mn-Doped and Nb-Doped CsPbCl<sub>3</sub> Monolayers as an Absorber Layer in Solar Cells. Journal of Physical Chemistry Letters, 2021, 12, 7319-7327. | 2.1 | 15 |
| 30 | Ab-initio investigation of crystal structure and pressure induced phase transition in ThO2 and PuO2. Materials Today Communications, 2021, 28, 102579. | 0.9 | 3 |
| 31 | Modulation of band gap and optical response of layered MoX2 (XÂ=ÂS, Se, Te) for electronic and optoelectronic applications. Materials Today Communications, 2021, 28, 102614. | 0.9 | 6 |
| 32 | Electric Field-Modulated Charge Transfer in Geometrically Tailored MoX<sub>2</sub>/WX<sub>2</sub> (X = S, Se) Heterostructures. Journal of Physical Chemistry C, 2021, 125, 22360-22369. | 1.5 | 15 |
| 33 | Highly selective and reversible 2D PtX2 (XÂ=ÂP, As) hazardous gas sensors: Ab-initio study. Applied Surface Science, 2021, 563, 150391. | 3.1 | 11 |
| 34 | Dissociation of air pollutants on the uniform surface of pentagonal BeP2. Applied Surface Science, 2021, 570, 151061. | 3.1 | 3 |
| 35 | Potential SiX (X = N, P, As, Sb, Bi) homo-bilayers for visible-light photocatalyst applications. Catalysis Science and Technology, 2021, 11, 4996-5013. | 2.1 | 18 |
| 36 | Metallic one-dimensional heterostructure for gas molecule sensing. Scientific Reports, 2021, 11, 433. | 1.6 | 2 |

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| 37 | Enhanced thermoelectric properties in Sb/Ge core/shell nanowires through vacancy modulation. Scientific Reports, 2021, 11, 21921. | 1.6 | 0 |
| 38 | Modulation of vertical strain and electric field on C3As/arsenene heterostructure. Applied Nanoscience (Switzerland), 2020, 10, 107-116. | 1.6 | 6 |
| 39 | First-principles study of the electronic, magnetic and optical properties of Fe3Se4 in its monoclinic phase. Journal of Magnetism and Magnetic Materials, 2020, 498, 166157. | 1.0 | 6 |
| 40 | Adsorption of toxic gas molecules on the pre-oxidized Cu2Si nanosheet â€“ A DFT study. Computational Materials Science, 2020, 173, 109414. | 1.4 | 41 |
| 41 | Structural and electrical properties of CeO2 monolayers using first-principles calculations. Solid State Communications, 2020, 307, 113801. | 0.9 | 12 |
| 42 | Synthesis and physicochemical characterization of rhamnolipid-stabilized carvacrol-loaded zein nanoparticles for antimicrobial application supported by molecular docking. Journal of Nanoparticle Research, 2020, 22, 1. | 0.8 | 23 |
| 43 | 2D BeP<sub>2</sub> monolayer: investigation of electronic and optical properties by driven modulated strain. RSC Advances, 2020, 10, 26804-26812. | 1.7 | 13 |
| 44 | Review: An insight into coronaviruses: Challenges, security and scope. Reviews in Medical Virology, 2020, 30, 1-8. | 3.9 | 6 |
| 45 | Ultrathin nanowire PdX<sub>2</sub> (X = P, As): stability, electronic transport and thermoelectric properties. New Journal of Chemistry, 2020, 44, 15617-15624. | 1.4 | 3 |
| 46 | Structural, optical, transport, and solar cell properties of 2D halide perovskite MAZX3 (Zâ€‰=â€‰Pb, Sn, and) Tj ETQq0 0 0 rgBT /Over | 1.1 | 18 |
| 47 | Rashba Splitting in Two Dimensional Hybrid Perovskite Materials for High Efficient Solar and Heat Energy Harvesting. Journal of Physical Chemistry Letters, 2020, 11, 7679-7686. | 2.1 | 14 |
| 48 | Elastic and thermal properties of terbium dihydride: An ab-initio study. AIP Conference Proceedings, 2020, , . | 0.3 | 2 |
| 49 | CdS/CdSe core/shell nanowire as cold anti-reflectors and high voltage nanodevices: A first principles study. AIP Conference Proceedings, 2020, , . | 0.3 | 0 |
| 50 | Transformation of electron density distribution induced by the cation point defects in uranium dioxide. Journal of Radioanalytical and Nuclear Chemistry, 2020, 325, 253-262. | 0.7 | 0 |
| 51 | Sputtering of material from the surface of PuO2 crystals by collision cascades impact. A molecular dynamics study. Nuclear Instruments & Methods in Physics Research B, 2020, 475, 39-43. | 0.6 | 4 |
| 52 | The impact of the collision cascades on the xenon and helium clusters in PuO2 crystals. A molecular dynamics simulation. Nuclear Instruments & Methods in Physics Research B, 2020, 476, 26-31. | 0.6 | 7 |
| 53 | Structural and electrical properties of ultrathin SiXC (X = 4, 5, 6) nanowires: A first principles calculation. AIP Conference Proceedings, 2020, , . | 0.3 | 0 |
| 54 | Correlation between experimental and theoretical study of scheelite and wolframite-type tungstates. Materials Today Communications, 2020, 25, 101417. | 0.9 | 4 |

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| 55 | Electronic structure and optical properties of Î²-CuSCN: A DFT study. Materials Today: Proceedings, 2020, 28, 164-167. | 0.9 | 15 |
| 56 | Metallic Sb/GaAs core/shell nanowire as cold anti-reflective coating for optical fibres. Materials Today: Proceedings, 2020, 28, 230-233. | 0.9 | 4 |
| 57 | Modulation of spin effect in electronic and vibrational properties of terbium dihydride (TbH2): An ab-initio study. International Journal of Hydrogen Energy, 2020, 45, 8783-8793. | 3.8 | 3 |
| 58 | Exploration of the strain and thermoelectric properties of hexagonal SiX (X = N, P, As, Sb, and Bi) monolayers. Physical Chemistry Chemical Physics, 2020, 22, 3990-3998. | 1.3 | 39 |
| 59 | A molecular simulation approach towards the development of universal nanocarriers by studying the pH- and electrostatic-driven changes in the dynamic structure of albumin. RSC Advances, 2020, 10, 13451-13459. | 1.7 | 11 |
| 60 | Lattice strain dependent optical properties of BaSnO3: First principle study. AIP Conference Proceedings, 2020, , . | 0.3 | 0 |
| 61 | Dimension dependent melting temperature of metallic nanoparticles. AIP Conference Proceedings, 2020, , . | 0.3 | 0 |
| 62 | Thermal conductivity of free-standing silicon nanowire using Raman spectroscopy. Nanotechnology, 2020, 31, 505701. | 1.3 | 4 |
| 63 | Quantum transport properties of Ni/Si nanowire for nano-electronic device application. AIP Conference Proceedings, 2019, , . | 0.3 | 1 |
| 64 | Influence of Li ion implantation on LO phonon broadening and bandgap opening in ZnO thin films. Journal of Alloys and Compounds, 2019, 806, 1138-1145. | 2.8 | 7 |
| 65 | Ab-initio study of strain engineering optical properties of RbPbI3. AIP Conference Proceedings, 2019, , . | 0.3 | 2 |
| 66 | Study of stability of 2D boron arsenide in air at atomic level. AIP Conference Proceedings, 2019, , . | 0.3 | 0 |
| 67 | Diameter dependency of characteristics of ultrathin Si nanowires. AIP Conference Proceedings, 2019, , . | 0.3 | 1 |
| 68 | Inquisitive Geometric Sites in h-BN Monolayer for Alkali Earth Metal Ion Batteries. Journal of Physical Chemistry C, 2019, 123, 19340-19346. | 1.5 | 18 |
| 69 | Effect of atomic order on the characteristic of SiGe nanowire. AIP Conference Proceedings, 2019, , . | 0.3 | 1 |
| 70 | Study of air stability mechanism of 2D boron antimonide. AIP Conference Proceedings, 2019, , . | 0.3 | 2 |
| 71 | High pressure cotunnite structure of ThO2: A DFT study. AIP Conference Proceedings, 2019, , . | 0.3 | 2 |
| 72 | Electronic and temperature dependent transport properties of ultrathin As and Sb nanowires. AIP Conference Proceedings, 2019, , . | 0.3 | 0 |

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| 73 | Study of interaction of nucleobases with ultrathin VO2 monoclinic nanowire. AIP Conference Proceedings, 2019, , . | 0.3 | 0 |
| 74 | The melting mechanisms of UO2 nanocrystals: A molecular dynamics simulation. AIP Conference Proceedings, 2019, , . | 0.3 | 1 |
| 75 | Stability and tunable electronic structure of planar phosphorus nanotubes. AIP Conference Proceedings, 2019, , . | 0.3 | 0 |
| 76 | Influence of defects on the diffusion of helium in uranium dioxide: Molecular dynamics study. AIP Conference Proceedings, 2019, , . | 0.3 | 2 |
| 77 | Energetic and structural investigation of thorium nanoclusters using first principles calculations. AIP Conference Proceedings, 2019, , . | 0.3 | 0 |
| 78 | Enhanced thermoelectric properties of BaReO3 perovskite by strain engineering. AIP Conference Proceedings, 2019, , . | 0.3 | 0 |
| 79 | Prospects for experimental realization of two-dimensional aluminium allotropes. Journal of Materials Chemistry C, 2019, 7, 2666-2675. | 2.7 | 24 |
| 80 | Two-dimensional silicon phosphide: low effective mass and direct band gap for future devices applications. Journal of Materials Science, 2019, 54, 11878-11888. | 1.7 | 14 |
| 81 | Spin polarization effect on the ground state and electronic properties of ErCu using DFT and DFT+U approaches. Physica B: Condensed Matter, 2019, 570, 122-127. | 1.3 | 5 |
| 82 | Surfactant prevented growth and enhanced thermophysical properties of CuO nanofluid. Journal of Molecular Liquids, 2019, 283, 550-557. | 2.3 | 33 |
| 83 | Computational study of electronic and optical properties of p-group atomic adsorption on Î±-Al2O3 (0001). Computational and Theoretical Chemistry, 2019, 1155, 101-108. | 1.1 | 5 |
| 84 | Structural, vibrational and optoelectronic properties of buckled metallic FeGe monolayer. Superlattices and Microstructures, 2019, 129, 62-68. | 1.4 | 3 |
| 85 | Two-Dimensional CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> with High Efficiency and Superior Carrier Mobility: A Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 5231-5239. | 1.5 | 41 |
| 86 | Energetic stability and tuned electronic properties of boron-doped carbon phosphide monolayer. AIP Conference Proceedings, 2019, , . | 0.3 | 0 |
| 87 | The influence of edge structure on the optoelectronic properties of Si2BN quantum dot. Journal of Applied Physics, 2019, 126, . | 1.1 | 17 |
| 88 | Effect of electric field on optoelectronic properties of indiene monolayer for photoelectric nanodevices. Scientific Reports, 2019, 9, 17300. | 1.6 | 18 |
| 89 | First principles study of stability and electronic properties of Sn/Ge core-shell nanowire. AIP Conference Proceedings, 2019, , . | 0.3 | 0 |
| 90 | Electronic structure of ZnO/CdX (X= S, Se, Te) core/shell nanowires: DFT study. AIP Conference Proceedings, 2019, , . | 0.3 | 3 |

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| 91 | Efficient and selective sensing of nitrogen-containing gases by Si2BN nanosheets under pristine and pre-oxidized conditions. Applied Surface Science, 2019, 469, 775-780. | 3.1 | 78 |
| 92 | Conjugation of biomolecules onto antimonene surface for biomedical prospects: A DFT study. Chemical Physics Letters, 2019, 715, 115-122. | 1.2 | 5 |
| 93 | Electronic structure and effective charges on atoms near anion point defects in uranium dioxide. Computational Condensed Matter, 2019, 18, e00353. | 0.9 | 1 |
| 94 | Dependence of Strain on the Electronic and Thermoelectric Properties of Hexagonal Bismuthene. Springer Proceedings in Physics, 2019, , 397-403. | 0.1 | 2 |
| 95 | Realization of Switching Mechanism of CO2 by Alkaline Adatoms on g-B4N3 Surface. Springer Proceedings in Physics, 2019, , 423-440. | 0.1 | 3 |
| 96 | Modulation of optical properties with multilayer thickness in antimonene and indieneÂ Â. Advanced Materials Letters, 2019, 10, 270-274. | 0.3 | 7 |
| 97 | Crystal Structure of AnO2 and Phase Transition at Higher Pressure: A Brief Review. Springer Proceedings in Physics, 2019, , 405-414. | 0.1 | 0 |
| 98 | Single layer of carbon phosphide as an efficient material for optoelectronic devices. Journal of Materials Science, 2018, 53, 8314-8327. | 1.7 | 41 |
| 99 | Effect on electronic and optical properties of Frenkel and Schottky defects in HfS2 monolayer. AIP Conference Proceedings, 2018, , . | 0.3 | 5 |
| 100 | Ab-initio study of thermodynamic properties of boron nanowire at atomic scale. AIP Conference Proceedings, 2018, , . | 0.3 | 0 |
| 101 | Improving electron transport in the hybrid perovskite solar cells using CaMnO3-based buffer layer. Nano Energy, 2018, 45, 287-297. | 8.2 | 19 |
| 102 | Boltzmann transport properties of ultra thin-layer of h-CX monolayers. AIP Conference Proceedings, 2018, , . | 0.3 | 0 |
| 103 | Ultrasonication effect on thermophysical properties of Al2O3 nanofluids. AIP Conference Proceedings, 2018, , . | 0.3 | 8 |
| 104 | Highly infrared sensitive VO<sub>2</sub> nanowires for a nano-optical device. Physical Chemistry Chemical Physics, 2018, 20, 11109-11115. | 1.3 | 11 |
| 105 | Electronic, Magnetic and Optical Properties of 2D Metal Nanolayers: A DFT Study. Metals and Materials International, 2018, 24, 904-912. | 1.8 | 6 |
| 106 | Effect of strain engineering on 2D dichalcogenides transition metal: A DFT study. Computational Materials Science, 2018, 141, 235-242. | 1.4 | 35 |
| 107 | Pressure-Dependent Electronic and Transport Properties of Bulk Platinum Oxide by Density Functional Theory. Journal of Electronic Materials, 2018, 47, 1293-1301. | 1.0 | 2 |
| 108 | Free-standing Pt and Pd nanowires: strain-modulated stability and magnetic and thermoelectric properties. Physical Chemistry Chemical Physics, 2018, 20, 28114-28123. | 1.3 | 6 |

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| 109 | Si and Ge based metallic core/shell nanowires for nano-electronic device applications. Scientific Reports, 2018, 8, 16885. | 1.6 | 18 |
| 110 | The effect of filler geometry on thermo-optical and rheological properties of CuO nanofluid. Journal of Molecular Liquids, 2018, 272, 668-675. | 2.3 | 21 |
| 111 | Ab-initio calculation on electronic and optical properties of ThO2, UO2 and PuO2. Journal of Nuclear Materials, 2018, 511, 128-133. | 1.3 | 20 |
| 112 | Î²-armchair antimony nanotube: Structure, stability and electronic properties. AIP Conference Proceedings, 2018, , . | 0.3 | 0 |
| 113 | Electronic and transport properties of 1D aluminum at atomic scale. AIP Conference Proceedings, 2018, , . | 0.3 | 1 |
| 114 | Tuning conductivity in boron nanowire by edge geometry. AIP Conference Proceedings, 2018, , . | 0.3 | 1 |
| 115 | Achieving ultrahigh carrier mobilities and opening the band gap in two-dimensional Si<sub>2</sub>BN. Physical Chemistry Chemical Physics, 2018, 20, 21716-21723. | 1.3 | 30 |
| 116 | First principles study of electronic structure and carrier mobility in Î²-armchair antimony nanotubes. Physics Letters, Section A: General, Atomic and Solid State Physics, 2018, 382, 2978-2983. | 0.9 | 4 |
| 117 | Catalytic activity of Cu4-cluster to adsorb H2S gas: h-BN nanosheet. AIP Conference Proceedings, 2018, , . | 0.3 | 3 |
| 118 | The electronic and optical properties of CH3NH3MoI3 perovskite. AIP Conference Proceedings, 2018, , . | 0.3 | 0 |
| 119 | Strain induced optical properties of BaReO3. AIP Conference Proceedings, 2018, , . | 0.3 | 2 |
| 120 | Strain induced structural and electronic properties of BaReO3: A DFT study. AIP Conference Proceedings, 2018, , . | 0.3 | 2 |
| 121 | Surfactant-assisted morphological studies of Î±-Al2O3 nanoparticles. AIP Conference Proceedings, 2018, , . | 0.3 | 1 |
| 122 | Reaction temperature dependent shape-controlled studies of copper-oxide nanocrystals. Materials Research Express, 2018, 5, 065037. | 0.8 | 8 |
| 123 | Theoretical Investigation of Metallic Nanolayers For Charge-Storage Applications. ACS Applied Energy Materials, 2018, 1, 3428-3433. | 2.5 | 19 |
| 124 | MgF 2 monolayer as an anti-reflecting material. Solid State Communications, 2017, 252, 22-28. | 0.9 | 27 |
| 125 | Structural, electronic and ferroelectric properties of BaTcO3. AIP Conference Proceedings, 2017, , . | 0.3 | 1 |
| 126 | Electronic and transport properties of fluorite structure of La2Ce2O7. AIP Conference Proceedings, 2017, , . | 0.3 | 1 |

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| 127 | Effect of oxygen atom on electronic and optical properties of 2D monolayer of PtS2. AIP Conference Proceedings, 2017, , . | 0.3 | 4 |
| 128 | Modeling of diameter-dependent Fe and Co ultrathin nanowires from first-principles calculations. Physical Chemistry Chemical Physics, 2017, 19, 15412-15423. | 1.3 | 17 |
| 129 | Spin dependent calculation of calcium manganese oxide. AIP Conference Proceedings, 2017, , . | 0.3 | 0 |
| 130 | Ab Initio Investigation of Vibrational, Optical and Thermodynamics Properties of Yttrium Arsenide. Journal of Electronic Materials, 2017, 46, 5670-5676. | 1.0 | 4 |
| 131 | Structural, electronic, mechanical and quantum transport of ultrathin gold nanowire: A density functional approach. Superlattices and Microstructures, 2017, 106, 206-215. | 1.4 | 9 |
| 132 | Review: Enhancing efficiency of solar thermal engineering systems by thermophysical properties of a promising nanofluids. Renewable and Sustainable Energy Reviews, 2017, 77, 1343-1348. | 8.2 | 19 |
| 133 | Experimental and theoretical analysis of electronic and optical properties of MgWO4. Journal of Materials Science, 2017, 52, 4934-4943. | 1.7 | 28 |
| 134 | Spin-dependent electron transport in C and Ge doped BN monolayers. Physical Chemistry Chemical Physics, 2017, 19, 30370-30380. | 1.3 | 7 |
| 135 | Modulating the electronic and optical properties of monolayer arsenene phases by organic molecular doping. Nanotechnology, 2017, 28, 495202. | 1.3 | 22 |
| 136 | Metal-Mott insulator transition of SrMnO3 by fluorine doping. AIP Conference Proceedings, 2017, , . | 0.3 | 1 |
| 137 | Oxygen adsorption on palladium monolayer as a surface catalyst. Physics Letters, Section A: General, Atomic and Solid State Physics, 2017, 381, 3084-3088. | 0.9 | 14 |
| 138 | High performance material for hydrogen storage: Graphenelike Si2BN solid. International Journal of Hydrogen Energy, 2017, 42, 22942-22952. | 3.8 | 50 |
| 139 | Structural, electronic and ferroelectric properties of BaReO3. AIP Conference Proceedings, 2017, , . | 0.3 | 2 |
| 140 | Re-solution of xenon clusters in plutonium dioxide under the collision cascade impact: A molecular dynamics simulation. AIP Conference Proceedings, 2017, , . | 0.3 | 1 |
| 141 | Temperature-dependent thermal conductivity and viscosity of synthesized Î±-alumina nanofluids. Applied Nanoscience (Switzerland), 2017, 7, 803-813. | 1.6 | 39 |
| 142 | A simulation of the helium diffusion in uranium dioxide crystals: a comparison of the interaction potentials. Bulletin of the Karaganda University Physics Series, 2017, 87, 26-30. | 0.1 | 3 |
| 143 | Molecular Dynamics Simulation of Xenon Diffusion in UO2 Nanocrystals. , 2017, , . | | 0 |
| 144 | Density functional Studies of structural, electronic and vibrational properties of palladium oxide. Solid State Communications, 2016, 245, 36-41. | 0.9 | 13 |

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| 145 | Ab-initio vibrational dynamics study of silver nanoclusters. AIP Conference Proceedings, 2016, , . | 0.3 | 1 |
| 146 | First-principles study of structural & electronic properties of pyramidal silicon nanowire. AIP Conference Proceedings, 2016, , . | 0.3 | 3 |
| 147 | Structural and opto-electronic properties of 2D AlSb monolayer. AIP Conference Proceedings, 2016, , . | 0.3 | 2 |
| 148 | First Principles Investigation of the Elastic, Optoelectronic and Thermal Properties of XRuSb: (XÂ=ÂV,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf<br>2016, 45, 3479-3490. | 1.0 | 46 |
| 149 | Germanene: a new electronic gas sensing material. RSC Advances, 2016, 6, 102264-102271. | 1.7 | 68 |
| 150 | First step to investigate nature of electronic states and transport in flower-like MoS2: Combining experimental studies with computational calculations. Scientific Reports, 2016, 6, 32690. | 1.6 | 20 |
| 151 | Photodynamic response of a solution-processed organolead halide photodetector. RSC Advances, 2016, 6, 111942-111949. | 1.7 | 4 |
| 152 | Ab-initio approach to IrO2 polymorphs â€“ properties at high pressures. AIP Conference Proceedings, 2016, , . | 0.3 | 0 |
| 153 | Antimonene: a monolayer material for ultraviolet optical nanodevices. Journal of Materials Chemistry C, 2016, 4, 6386-6390. | 2.7 | 246 |
| 154 | 2D-HfS<sub>2</sub>as an efficient photocatalyst for water splitting. Catalysis Science and Technology, 2016, 6, 6605-6614. | 2.1 | 71 |
| 155 | Indiene 2D monolayer: a new nanoelectronic material. RSC Advances, 2016, 6, 8006-8014. | 1.7 | 45 |
| 156 | Elasticity of DNA nanowires. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 207-210. | 0.9 | 8 |
| 157 | Temperature and Size Dependent Thermal Conductivity of Graphene Nanoribbons Description for Phonon Dispersion and Polarization. Advanced Science Letters, 2016, 22, 3916-3918. | 0.2 | 2 |
| 158 | Length, width and roughness dependent thermal conductivity of graphene nanoribbons. Chemical Physics Letters, 2015, 634, 16-19. | 1.2 | 39 |
| 159 | Size and edge roughness effects on thermal conductivity of pristine antimonene allotropes. Chemical Physics Letters, 2015, 641, 169-172. | 1.2 | 60 |
| 160 | Evidence of a graphene-like Sn-sheet on a Au(111) substrate: electronic structure and transport properties from first principles calculations. Physical Chemistry Chemical Physics, 2015, 17, 6705-6712. | 1.3 | 33 |
| 161 | Interaction of metallic clusters with biologically active curcumin molecules. Chemical Physics Letters, 2015, 636, 163-166. | 1.2 | 0 |
| 162 | Modulation of band gap by an applied electric field in silicene-based hetero-bilayers. Physical Chemistry Chemical Physics, 2015, 17, 11324-11328. | 1.3 | 58 |

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| 163 | Unique electron transport in ultrathin black phosphorene: Ab-initio study. Applied Surface Science, 2015, 356, 881-887. | 3.1 | 33 |
| 164 | Step energy and step interactions on the reconstructed GaAs(001) surface. Physical Review B, 2014, 90, . | 1.1 | 7 |
| 165 | Zeolite-Y entrapped bivalent transition metal complexes as hybrid nanocatalysts: density functional theory investigation and catalytic aspects. Green Chemistry Letters and Reviews, 2014, 7, 278-287. | 2.1 | 36 |
| 166 | Structural, electronic, optical and thermodynamic properties of cubic REGa3 (RE=Sc or Lu) compounds: Ab initio study. Journal of Alloys and Compounds, 2014, 597, 36-44. | 2.8 | 57 |
| 167 | Nature of low compressibility and anisotropic elasticity in YbB2. Journal of Alloys and Compounds, 2014, 597, 148-154. | 2.8 | 3 |
| 168 | First-principles studies of the superconductivity and vibrational properties of transition-metal nitrides TMN (TMÂ=ÂTi, V, and Cr). Materials Chemistry and Physics, 2014, 143, 503-513. | 2.0 | 27 |
| 169 | A comparative study of experimental and theoretical results of conformations of oxovanadium(IV) complexes with 4-acyl pyrazolone ligands using DFT method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 447-451. | 2.0 | 5 |
| 170 | Effect of Si doping on the electronic properties of BN monolayer. Nanoscale, 2014, 6, 5526-5531. | 2.8 | 42 |
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