# Ali Hussain Reshak

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 454 papers | 9,926 citations | 45 h-index | 75 g-index |
| 473 ext. papers | 11,143 ext. citations | 3.8 avg, IF | 6.99 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 454 | Cationic variation for LnAl2Si2 (Ln´=´Y, Sm, Tb, Dy, Yb) compounds by density functional theory. *Journal of Molecular Structure*, **2022**, 1252, 132136 | 3.4 | 0 |
| 453 | Dielectric absorption correlated to ferromagnetic behavior in (Cr, Ni)-codoped 4HSiC for microwave applications. *Journal of Molecular Structure*, **2022**, 1248, 131462 | 3.4 | 9 |
| 452 | Thermoelectric, structural, electronic, magnetic, and thermodynamic properties of CaZn2Ge2 compound. *European Physical Journal Plus*, **2022**, 137, 1 | 3.1 | 0 |
| 451 | Effects of anion-ligands replacement on the Structural, Electronic and Magnetic properties of ThCo2X2 (X´=´Si, Ge). *Chinese Journal of Physics*, **2022**, 77, 956-964 | 3.5 | 0 |
| 450 | Bismuth-containing semiconductors GaAs1−xBix for energy conversion: Thermoelectric properties. *Materials Science in Semiconductor Processing*, **2022**, 148, 106850 | 4.3 | 2 |
| 449 | Computational investigation of structural, magnetic, elastic, and electronic properties of Half-Heusler ScVX (X = Si, Ge, Sn, and Pb) compounds. *European Physical Journal Plus*, **2021**, 136, 1 | 3.1 | 1 |
| 448 | First-principles calculations of structural, electronic, optical, and thermoelectric properties of ternary d-metal sulfides Sc2CdS4 and Y2CdS4 compounds. *International Journal of Energy Research*, **2021**, 45, 13657-13667 | 4.5 | 1 |
| 447 | Strain effect on the electronic and optical properties of 2D Tetrahexcarbon: a DFT-based study. *Indian Journal of Physics*, **2021**, 95, 2365 | 1.4 | 11 |
| 446 | CoYZ (Y= Cr, Nb, Ta, V and Z= Al, Ga) Heusler alloys under the effect of pressure and strain. *Journal of Molecular Graphics and Modelling*, **2021**, 104, 107841 | 2.8 | 14 |
| 445 | Coupling ferroelectric polarization and anisotropic charge migration for enhanced CO2 photoreduction. *Applied Catalysis B: Environmental*, **2021**, 284, 119709 | 21.8 | 22 |
| 444 | Insight into the physical properties of the inter-metallic titanium-based binary compounds. *European Physical Journal Plus*, **2021**, 136, 1 | 3.1 | 14 |
| 443 | Structural, electronic and optoelectronic properties of AB5C8 (A = Cu/Ag; B = In and C = S, Se and Te) compounds. *International Journal of Energy Research*, **2021**, 45, 4014-4025 | 4.5 | 1 |
| 442 | Genesis of magnetism in graphene/MoS2 van der Waals heterostructures via interface engineering using Cr-adsorption. *Journal of Alloys and Compounds*, **2021**, 859, 157776 | 5.7 | 13 |
| 441 | Optoelectronic and transport properties of Rb/Cs2TeI6 defective perovskites for green energy applications. *International Journal of Energy Research*, **2021**, 45, 8448-8455 | 4.5 | 7 |
| 440 | Pressure-dependent elasto-mechanical stability and thermoelectric properties of MYbF3 (M = Rb, Cs) materials for renewable energy. *International Journal of Energy Research*, **2021**, 45, 8711-8723 | 4.5 | 13 |
| 439 | Modeling Complex Systems by Structural Invariants Approach. *Complexity*, **2021**, 2021, 1-17 | 1.6 | |
| 438 | 2D Hexagonal SnTe monolayer: a quasi direct band gap semiconductor with strain sensitive electronic and optical properties. *European Physical Journal B*, **2020**, 93, 1 | 1.2 | 4 |

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| 437 | Mechanical stability and optoelectronic behavior of BeXP2 (X=Si and Ge) chalcopyrite. *Chinese Journal of Physics*, **2020**, 64, 174-182 | 3.5 | 9 |
| 436 | Magnetism and magnetocrystalline anisotropy of tetragonally distorted L10-FeNi: N alloy. *Journal of Alloys and Compounds*, **2020**, 835, 155325 | 5.7 | 6 |
| 435 | Phase Transition as an Emergent Phenomenon Analysed by Violation of Structural Invariant (M, BM). *Mendel*, **2020**, 26, 45-50 | 1.4 | 2 |
| 434 | Optical features of novel semiconducting crystals Tl1−xGa1−xSnxSe2 (x=0.05; 0.1). *Optik*, **2020**, 206, 163572 | 2.5 | |
| 433 | Structural, elastic, electronic, magnetic, optical, and thermoelectric properties of the diamond-like quaternary semiconductor CuMn2InSe4. *Journal of Superconductivity and Novel Magnetism*, **2020**, 33, 1091-1102 | 1.5 | 25 |
| 432 | Laser-stimulated Pockels effect in CdBr2/Cu polymer nanocomposites. *Physica E: Low-Dimensional Systems and Nanostructures*, **2020**, 118, 113904 | 3 | 0 |
| 431 | Pressure induced physical variations in the lead free fluoropervoskites XYF3 (X=K, Rb, Ag; Y=Zn, Sr, Mg): Optical materials. *Optical Materials*, **2020**, 109, 110325 | 3.3 | 4 |
| 430 | Structural, electronic and thermoelectric properties of topological semimetal lanthanum monopnicitide LaBi. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2020**, 384, 126789 | 2.3 | 2 |
| 429 | Structural, electronic and magnetic properties of new full Heusler alloys Rh2CrZ (Z = Al, Ga, In): First-principles calculations. *Chinese Journal of Physics*, **2019**, 59, 281-290 | 3.5 | 15 |
| 428 | First principles prediction of the elastic, electronic and optical properties of Sn3X4 (X = P, As, Sb, Bi) compounds: Potential photovoltaic absorbers. *Chinese Journal of Physics*, **2019**, 59, 265-272 | 3.5 | 4 |
| 427 | Novel dibenzothiophene chromophores with peripheral barbituric acceptors. *Tetrahedron*, **2019**, 75, 130459 | 2.4 | 6 |
| 426 | Untangling electronic, optical and bonding properties of hexagonal bismuth borate SrBi2B2O7 crystal for ultraviolet opto-electronic applications: An ab initio study. *Journal of Alloys and Compounds*, **2019**, 803, 1127-1135 | 5.7 | 6 |
| 425 | Specific features of 3, 6-bis (4-hydroxy phenyl)-piperazine-2, 5-dione (BHPPD) diphenolic monomer and compered with toxic industrial bisphenol-A (BPA): DFT calculation. *Materials Chemistry and Physics*, **2019**, 236, 121780 | 4.4 | 10 |
| 424 | Noncentrosymmetric Sulfide Oxide MZnSO (M = Ca or Sr) with Strongly Polar Structure as Novel Nonlinear Crystals. *Journal of Physical Chemistry C*, **2019**, 123, 27172-27180 | 3.8 | 21 |
| 423 | Phase transition in BaThO3 from Pbnm to Ibmm turn the fundamental energy band gap from indirect to direct. *Journal of Alloys and Compounds*, **2019**, 771, 607-613 | 5.7 | 8 |
| 422 | Ferroelectric polarization promoted bulk charge separation for highly efficient CO2 photoreduction of SrBi4Ti4O15. *Nano Energy*, **2019**, 56, 840-850 | 17.1 | 95 |
| 421 | Electronic, bonding and optical properties of the LiGaGe2X6 (X = S, Se, and Te) compounds: An ab initio study. *Optik*, **2019**, 180, 782-791 | 2.5 | 1 |
| 420 | Chairlike and Boatlike Graphane: Active Photocatalytic Water Splitting Solar-to-Hydrogen Energy Conversion under UV Irradiation. *Journal of Physical Chemistry C*, **2018**, 122, 8076-8081 | 3.8 | 8 |

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| 419 | Effect of Si and Ge Surface Doping on the Be2C Monolayer: Case Study on Electrical and Optical Properties. *Silicon*, **2018**, 10, 1893-1902 | 2.4 | 2 |
| 418 | Electronic, bonding, linear, and nonlinear optical properties of Na 2 MGe 2 Q 6 (M=Cd, Zn, Hg; Q=S, Se), Na 2 ZnSi 2 S 6 , and Na 2 ZnSn 2 S 6 two metal-mixed chalcogenide compounds: Insights from an ab initio study. *Journal of Physics and Chemistry of Solids*, **2018**, 119, 220-227 | 3.9 | 13 |
| 417 | Novel photocatalytic water splitting solar-to-hydrogen energy conversion: CdLaS and CdLaSe ternary semiconductor compounds. *Physical Chemistry Chemical Physics*, **2018**, 20, 8848-8858 | 3.6 | 10 |
| 416 | A novel photocatalytic water splitting solar-to-hydrogen energy conversion: Non-centro-symmetric borate CsZn2B3O7 photocatalyst. *Journal of Alloys and Compounds*, **2018**, 741, 1258-1268 | 5.7 | 10 |
| 415 | One- and two-dimensional search of an equation of state using a newly released 2DRoptimize package. *Journal of Physics and Chemistry of Solids*, **2018**, 116, 131-136 | 3.9 | 3 |
| 414 | Visible-Light-Responsive Sill□-Structured Mixed-Cationic CdBiO2Br Nanosheets: Layer Structure Design Promoting Charge Separation and Oxygen Activation Reactions. *Journal of Physical Chemistry C*, **2018**, 122, 2661-2672 | 3.8 | 51 |
| 413 | Fabrication and Characterization of a p-AgO/PSi/n-Si Heterojunction for Solar Cell Applications. *Silicon*, **2018**, 10, 371-376 | 2.4 | 12 |
| 412 | Active photocatalytic water splitting solar-to-hydrogen energy conversion: Chalcogenide photocatalyst Ba2ZnSe3 under visible irradiation. *Applied Catalysis B: Environmental*, **2018**, 221, 17-26 | 21.8 | 33 |
| 411 | Synthesis, Crystal Structure, and Optical Gap of Two-Dimensional Halide Solid Solutions CsPb(ClBr ). *Inorganic Chemistry*, **2018**, 57, 9531-9537 | 5.1 | 9 |
| 410 | Insight into crystal-structure dependent charge separation and photo-redox catalysis: A combined experimental and theoretical study on Bi(IO3)3 and BiOIO3. *Applied Surface Science*, **2018**, 458, 129-138 | 6.7 | 19 |
| 409 | AA- and ABA-stacked carbon nitride (CN): novel photocatalytic water splitting solar-to-hydrogen energy conversion. *Physical Chemistry Chemical Physics*, **2018**, 20, 22972-22979 | 3.6 | 5 |
| 408 | Sulfide oxide XZnSO (X = Ca or Sr) as novel active photocatalytic water splitting solar-to-hydrogen energy conversion. *Applied Catalysis B: Environmental*, **2018**, 225, 273-283 | 21.8 | 16 |
| 407 | Synthesis and Characterization of Cu2CdSnS4 Quaternary Alloy Nanostructures. *International Journal of Electrochemical Science*, **2018**, 6693-6707 | 2.2 | 19 |
| 406 | Electronic structure and optical properties of dilute boron-bismide quaternary alloys B Ga1□As1□Bi /GaAs for infrared optoelectronic devices. *Optik*, **2017**, 135, 57-69 | 2.5 | 9 |
| 405 | Electronic structure and optical properties of □RbSm(MoO 4 ) 2 from spin polarization calculations: DFT+U. *Materials Chemistry and Physics*, **2017**, 192, 260-267 | 4.4 | 3 |
| 404 | Structure stability and magnetism in graphene impurity complexes with embedded V and Nb atoms. *Journal of Magnetism and Magnetic Materials*, **2017**, 433, 109-115 | 2.8 | 8 |
| 403 | Synthesis, Structural, Thermal, and Electronic Properties of Palmierite-Related Double Molybdate □CsPb(MoO). *Inorganic Chemistry*, **2017**, 56, 3276-3286 | 5.1 | 30 |
| 402 | The influence of oxygen vacancies on the linear and nonlinear optical properties of Pb7O(OH)3(CO3)3(BO3). *RSC Advances*, **2017**, 7, 14752-14760 | 3.7 | 24 |

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| 401 | Spin-polarized antiferromagnetic CaCoSO single crystal: First-principles study. *Journal of Alloys and Compounds*, **2017**, 711, 229-234 | 5.7 | 1 |
| 400 | Spin-polarized Second Harmonic Generation from the Antiferromagnetic CaCoSO Single Crystal. *Scientific Reports*, **2017**, 7, 46415 | 4.9 | 116 |
| 399 | Electronic, optical, and thermoelectric properties of Fe2+xV1−xAl. *AIP Advances*, **2017**, 7, 045118 | 1.5 | 22 |
| 398 | Photocatalytic water splitting solar-to-hydrogen energy conversion: Perovskite-type hydride XBeH 3 (X = Li or Na) as active photocatalysts. *Journal of Catalysis*, **2017**, 351, 119-129 | 7.3 | 12 |
| 397 | The under-pressure behaviour of mechanical, electronic and optical properties of calcium titanate and its ground state thermoelectric response. *Philosophical Magazine*, **2017**, 97, 1884-1901 | 1.6 | 38 |
| 396 | Photocatalytic water-splitting solar-to-hydrogen energy conversion: Novel LiMoO 3 (IO 3 ) molybdenyl iodate based on WO 3 -type sheets. *Journal of Catalysis*, **2017**, 351, 1-9 | 7.3 | 9 |
| 395 | Electronic and optical properties of pentagonal-B2C monolayer: A first-principles calculation. *International Journal of Modern Physics B*, **2017**, 31, 1750044 | 1.1 | 22 |
| 394 | CaCoSO diluted magnetic antiferromagnet semiconductor as efficient thermoelectric materials. *Materials Research Bulletin*, **2017**, 94, 22-30 | 5.1 | 1 |
| 393 | Revealing the transport properties of the spin-polarized β-Tb 2 (MoO 4 ) 3 : DFT+U. *Journal of Magnetism and Magnetic Materials*, **2017**, 441, 124-130 | 2.8 | |
| 392 | Photophysical, transport and structure properties of Tl10Hg3Cl16 single crystals: Novel photocatalytic water-splitting solar-to-hydrogen energy conversion. *Journal of Catalysis*, **2017**, 352, 142-154 | 7.3 | 9 |
| 391 | Novel borate CsZn2B3O7 single crystal with large efficient second harmonic generation in deep-ultraviolet spectral range. *Journal of Alloys and Compounds*, **2017**, 722, 438-444 | 5.7 | 23 |
| 390 | Highly desirable semiconducting materials for mid-IR optoelectronics: Dilute bismide InAs1−xBix alloys. *Materials Research Bulletin*, **2017**, 95, 588-596 | 5.1 | 13 |
| 389 | Electronic and optical properties of paratellurite TeO2 under pressure: A first-principles calculation. *Optik*, **2017**, 139, 9-15 | 2.5 | 16 |
| 388 | Comparative first-principles calculations of the electronic, optical, elastic and thermodynamic properties of XCaF3 (X = K, Rb, Cs) cubic perovskites. *Materials Chemistry and Physics*, **2017**, 188, 39-48 | 4.4 | 18 |
| 387 | Role of spin-orbit interaction on the nonlinear optical response of CsPbCOF using DFT. *Physical Chemistry Chemical Physics*, **2017**, 19, 31255-31266 | 3.6 | 16 |
| 386 | Lithium borate LiBO(OH) with large second harmonic generation and a high damage threshold in the deep-ultraviolet spectral range. *Physical Chemistry Chemical Physics*, **2017**, 19, 30703-30714 | 3.6 | 9 |
| 385 | Novel ternary semiconductor CdLa2X4 (X=S or Se) single crystal with efficient second harmonic generation in the visible spectral range. *Journal of Alloys and Compounds*, **2017**, 728, 241-252 | 5.7 | 9 |
| 384 | Quantum dots in photocatalytic applications: efficiently enhancing visible light photocatalytic activity by integrating CdO quantum dots as sensitizers. *Physical Chemistry Chemical Physics*, **2017**, 19, 24915-24927 | 3.6 | 27 |

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| 383 | Macroscopic Polarization Enhancement Promoting Photo- and Piezoelectric-Induced Charge Separation and Molecular Oxygen Activation. *Angewandte Chemie - International Edition*, **2017**, 56, 11860-11864 | 16.4 | 662 |
| 382 | Formation of metastable phases of ferrous sulfide via pulsed Nd:YAG laser deposition: Experimental and theoretical study. *Journal of Alloys and Compounds*, **2017**, 723, 689-697 | 5.7 | 3 |
| 381 | Two haloid borate crystals with large nonlinear optical response. *Physical Chemistry Chemical Physics*, **2017**, 19, 18416-18425 | 3.6 | 13 |
| 380 | First-Principles Study on the Structural, Electronic, Magnetic and Thermodynamic Properties of Full Heusler Alloys Co2VZ (Z = Al, Ga). *Journal of Electronic Materials*, **2017**, 46, 130-142 | 1.9 | 21 |
| 379 | Chlorine intercalation in graphitic carbon nitride for efficient photocatalysis. *Applied Catalysis B: Environmental*, **2017**, 203, 465-474 | 21.8 | 241 |
| 378 | Thermoelectric properties of TbFe2 and TbCo2 in C15- laves phase: Spin-polarized DFT+U approach. *Journal of Magnetism and Magnetic Materials*, **2017**, 422, 287-298 | 2.8 | 8 |
| 377 | Metal Hydrides: Electronic Band Structure **2017**, | | |
| 376 | Exploring the electronic structure of Pb 2+ ions containing material Pb 16 (OH) 16 (NO 3 ) 16. *Journal of Physics and Chemistry of Solids*, **2016**, 99, 75-81 | 3.9 | 1 |
| 375 | Transport properties of the n-type SrTiO3/LaAlO3 interface. *RSC Advances*, **2016**, 6, 92887-92895 | 3.7 | 6 |
| 374 | Revealing the electronic structure and optical properties of K6[Mo4O8F10] novel molybdenum oxyfluoride materials. *Philosophical Magazine*, **2016**, 96, 3131-3142 | 1.6 | 1 |
| 373 | Thermoelectric Properties of the Intermetallic Quasi-Two-Dimensional Layered Structure LiBe. *Journal of Electronic Materials*, **2016**, 45, 5546-5553 | 1.9 | |
| 372 | First-principles investigation of the optical properties for rocksalt mixed metal oxide MgxZn1−xO. *Materials Chemistry and Physics*, **2016**, 182, 182-189 | 4.4 | 14 |
| 371 | Electronic structure, first and second order physical properties of MPS4: a theoretical study. *Materials Science-Poland*, **2016**, 34, 275-285 | 0.6 | 2 |
| 370 | Experimental and theoretical study of the electronic structure and optical spectral features of PbIn6Te10. *RSC Advances*, **2016**, 6, 73107-73117 | 3.7 | 5 |
| 369 | Thermoelectric properties of the spin-polarized half-metallic ferromagnetic CsTe and RbSe compounds. *RSC Advances*, **2016**, 6, 98197-98207 | 3.7 | 8 |
| 368 | Revealing the structural, elastic and thermodynamic properties of CdSexTe1−x (x´=´0, 0.25, 0.5, 0.75, 1). *Journal of Alloys and Compounds*, **2016**, 667, 151-157 | 5.7 | 8 |
| 367 | LiMoO3(IO3), a novel molybdenyl iodate with strong second-order optical nonlinearity. *Journal of Alloys and Compounds*, **2016**, 660, 32-38 | 5.7 | 5 |
| 366 | DFT calculations for the electronic structure of alpha phase of CsMgH3 as advanced hydrogen storage materials. *International Journal of Hydrogen Energy*, **2016**, 41, 2762-2770 | 6.7 | 6 |

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| 365 | Comparative study of Fe doped ZnO based diluted and condensed magnetic semiconductors in wurtzite and zinc-blende structures by first-principles calculations. *Materials Science in Semiconductor Processing*, **2016**, 43, 123-128 | 4.3 | 19 |
| 364 | Realization and computational analysis of splitting in higher order optical vortices. *Optik*, **2016**, 127, 5757-5760 | 2.5 | 1 |
| 363 | Evanescent field optimization on Y-branch silicon nitride optical waveguide for biosensing. *Materials Letters*, **2016**, 173, 127-130 | 3.3 | 1 |
| 362 | Strong second harmonic generation in LiInX2 (X=Se, Te) chalcopyrite crystals as explored by first-principles methods. *Journal of Alloys and Compounds*, **2016**, 675, 355-363 | 5.7 | 15 |
| 361 | Electronic structure and transport properties of Ba2Cd2Pn3 (Pn = As and Sb): An efficient materials for energy conversion. *Journal of Alloys and Compounds*, **2016**, 670, 1-11 | 5.7 | 8 |
| 360 | Influence of an oxygen vacancy on the electronic structure of the asymmetric mixed borate–carbonate Pb7O(OH)3(CO3)3(BO3). *RSC Advances*, **2016**, 6, 18965-18972 | 3.7 | 1 |
| 359 | Investigation of structural, electronic, and optical properties of the monoclinic and triclinic polymorphs of hexamethylenetetraminium 2,4-dinitrophenolate monohydrate (C6H13N4+·C6H3N2O5−·H2O) compound: A DFT approach. *Materials Chemistry and Physics*, **2016**, 172, 77-86 | 4.4 | 2 |
| 358 | Structural and electronic properties of InNxP1-x alloy in full range (0 ≤ x ≤ 1). *Philosophical Magazine*, **2016**, 96, 991-1005 | 1.6 | 3 |
| 357 | Half metallicity and magnetism in graphene containing monovacancies decorated with Carbon/Nitrogen adatom. *Journal of Alloys and Compounds*, **2016**, 663, 100-106 | 5.7 | 12 |
| 356 | Quest for magnetism in graphene via Cr- and Mo-doping: A DFT approach. *Physica E: Low-Dimensional Systems and Nanostructures*, **2016**, 78, 35-40 | 3 | 24 |
| 355 | Spin-polarization in filled-skutterudites LaFe 4 Pn 12 ( Pn =P, As and Sb). *Journal of Magnetism and Magnetic Materials*, **2016**, 401, 684-694 | 2.8 | 3 |
| 354 | Revealing the influence of the compression mechanism on the electronic structure and the related properties of CrF 3. *Journal of Alloys and Compounds*, **2016**, 660, 1-10 | 5.7 | 1 |
| 353 | Structural, optical and electrical properties of Cu2Zn1−xCdxSnS4 quinternary alloys nanostructures deposited on porous silicon. *Microsystem Technologies*, **2016**, 22, 2893-2900 | 1.7 | 16 |
| 352 | Electronic and optical properties of α-Tb2(MoO4)3: DFT+U approach. *European Physical Journal B*, **2016**, 89, 1 | 1.2 | 1 |
| 351 | Lead nitrate hydroxide: A strong second-order optical nonlinearity acentric crystal with high laser damage thresholds. *Journal of Applied Physics*, **2016**, 119, 105706 | 2.5 | 6 |
| 350 | Revealing the origin of the strong second harmonic generation of Li2CdXS4 and Li2CdXS4 (X = Ge or Sn). *Journal of Applied Physics*, **2016**, 119, 095709 | 2.5 | 3 |
| 349 | Two symmetric n-type interfaces SrTiO3/LaAlO3 in perovskite: Electronic properties from density functional theory. *Journal of Applied Physics*, **2016**, 119, 245303 | 2.5 | 25 |
| 348 | Revealing the spin-polarized optical properties of monoclinic Eu2(MoO4)3: a DFT + U approach. *RSC Advances*, **2016**, 6, 51675-51682 | 3.7 | 2 |

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| 347 | Transport properties of Co-based Heusler compounds Co2VAl and Co2VGa: spin-polarized DFT+U. *RSC Advances*, **2016**, 6, 54001-54012 | 3.7 | 20 |
| 346 | Exploration of the Electronic Structure of Monoclinic Eu2(MoO4)3: DFT-Based Study and X-ray Photoelectron Spectroscopy. *Journal of Physical Chemistry C*, **2016**, 120, 10559-10568 | 3.8 | 52 |
| 345 | Effect of lead and caesium on the mechanical, vibrational and thermodynamic properties of hexagonal fluorocarbonates: a comparative first principles study. *RSC Advances*, **2016**, 6, 99885-99897 | 3.7 | 11 |
| 344 | Thermoelectric properties of highly-mismatched alloys of GaNxAs1 from first- to second-principles methods: energy conversion. *RSC Advances*, **2016**, 6, 72286-72294 | 3.7 | 21 |
| 343 | Theoretical investigation of the structural, electronic, magnetic and elastic properties of binary cubic C15-Laves phases TbX2 (X = Co and Fe). *Journal of Alloys and Compounds*, **2016**, 689, 885-893 | 5.7 | 23 |
| 342 | Structural investigations through cobalt effect on ZnO nanostructures. *Optik*, **2016**, 127, 10102-10107 | 2.5 | 19 |
| 341 | Single Brillouin frequency shifted S-band multi-wavelength Brillouin-Raman fiber laser utilizing fiber Bragg grating and Raman amplifier in ring cavity. *Optical Materials*, **2016**, 60, 38-44 | 3.3 | 2 |
| 340 | Specific features of electronic structures and optical susceptibilities of molybdenum oxide. *RSC Advances*, **2015**, 5, 22044-22052 | 3.7 | 40 |
| 339 | First-principles calculation on dilute magnetic alloys in zinc blend crystal structure. *Journal of Magnetism and Magnetic Materials*, **2015**, 385, 27-31 | 2.8 | 9 |
| 338 | Theoretical study of the new zintl phases compounds K2ACdSb2 (A=(Sr, Ba)). *Physica B: Condensed Matter*, **2015**, 464, 9-16 | 2.8 | |
| 337 | Ab initio method of optical investigations of CdS 1x Te x alloys under quantum dots diameter effect. *Solar Energy*, **2015**, 115, 33-39 | 6.8 | 40 |
| 336 | Experimental and theoretical investigation of the electronic structure and optical properties of TlHgCl3 single crystal. *Optical Materials*, **2015**, 47, 445-452 | 3.3 | 6 |
| 335 | Specific features of the electronic structure and optical properties of skutterudites LaFe4X12 (X=P, As and Sb). *Optical Materials*, **2015**, 47, 453-461 | 3.3 | 4 |
| 334 | Electronic structure of alkali-metal/alkaline-earth-metal fluorine beryllium borate NaSr3Be3B3O9F4 single crystal: DFT approach. *Optical Materials*, **2015**, 48, 25-30 | 3.3 | 1 |
| 333 | Theoretical investigation of some specific features of the electronic structure and optical properties of Benzoic Acid 2-Amino-4,6-Dimethylpyrimidine (1:1) co-crystals. *Optical Materials*, **2015** , 46, 216-222 | 3.3 | 4 |
| 332 | Mixed alkali and alkaline-earth borate Li2Sr4B12O23 single crystal. *Optical Materials*, **2015**, 48, 165-171 | 3.3 | |
| 331 | The influence of replacing the pnicogens As by Sb on the optical properties of the Zintl phases Ba2Cd2Pn3 (Pn´=´As and Sb). *Journal of Alloys and Compounds*, **2015**, 648, 1-6 | 5.7 | 2 |
| 330 | Generating magnetic response and half-metallicity in GaP via dilute Ti-doping for spintronic applications. *Journal of Alloys and Compounds*, **2015**, 649, 184-189 | 5.7 | 15 |

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| 329 | Thermoelectric properties of fully hydrogenated graphene: Semi-classical Boltzmann theory. *Journal of Applied Physics*, **2015**, 117, 225104 | 2.5 | 13 |
| 328 | Nowotny□uza NaZnX (X = P, As and Sb) as photovoltaic materials. *Solar Energy*, **2015**, 115, 430-440 | 6.8 | 3 |
| 327 | Non-centrosymmetric LiBaB9O15 single crystal: growth and characterization. *Indian Journal of Physics*, **2015**, 89, 923-929 | 1.4 | 2 |
| 326 | Microcrystalline □RbNd(MoO4)2: spin polarizing DFT+U. *RSC Advances*, **2015**, 5, 44960-44968 | 3.7 | 6 |
| 325 | Transport properties of g-BC3 and t-BC3 phases. *RSC Advances*, **2015**, 5, 33632-33638 | 3.7 | 24 |
| 324 | Specific features of electronic structures and optical susceptibilities of g-BC3 and t-BC3 phases. *Physical Chemistry Chemical Physics*, **2015**, 17, 8006-16 | 3.6 | 6 |
| 323 | Engineering oxygen vacancies towards self-activated BaLuAl(x)Zn(4-x)O(7-(1-x)/2) photoluminescent materials: an experimental and theoretical analysis. *Physical Chemistry Chemical Physics*, **2015**, 17, 31188-94 | 3.6 | 36 |
| 322 | Alkali-metal/alkaline-earth-metal fluorine beryllium borate NaSr3Be3B3O9F4 with large nonlinear optical properties in the deep-ultraviolet region. *Journal of Applied Physics*, **2015**, 117, 085703 | 2.5 | 30 |
| 321 | Second harmonic generation from the novel polar polymorph □BaTeMo2O9 phases. *RSC Advances*, **2015**, 5, 70992-71001 | 3.7 | 1 |
| 320 | Enhanced magnetic response and metallicity in AB stacked bilayer graphene via Cr-doping. *Journal of Alloys and Compounds*, **2015**, 649, 1300-1305 | 5.7 | 13 |
| 319 | Effect of X on the transport properties of skutterudites LaFe 4 X 12 (X´=´P, As and Sb) compounds. *Journal of Alloys and Compounds*, **2015**, 651, 176-183 | 5.7 | 2 |
| 318 | The electronic band structure of polar polymorph □BaTeMo2O9 phases. *Journal of Alloys and Compounds*, **2015**, 651, 308-315 | 5.7 | 1 |
| 317 | From micro-to macroscopic: Understanding optical properties in zinc-blend-derived materials Cu2ZnYX4(X´=´S, Se, Te, Y´=´Si, Ge, Sn) by means of the quantum chemical topology analysis. *Journal of Alloys and Compounds*, **2015**, 653, 140-147 | 5.7 | 6 |
| 316 | Thermoelectric properties of Sr+1Ti O3+1 (n=1, 2, 3, □Ruddlesden□Popper Homologous Series. *Renewable Energy*, **2015**, 76, 36-44 | 8.1 | 18 |
| 315 | Transport properties of mixed CuAl(S1□Sex)2 as promising thermoelectric crystalline materials. *Journal of Physics and Chemistry of Solids*, **2015**, 78, 46-52 | 3.9 | 21 |
| 314 | Thermoelectric, electronic, optical and chemical bonding properties of Ba2PrRuO6: At temperature 7 K and 150 K. *Materials Research Bulletin*, **2015**, 61, 551-559 | 5.1 | 2 |
| 313 | First principles treatment of structural, optical, and thermoelectric properties of Li7MnN4 as electrode for a Li secondary battery. *Materials Research Bulletin*, **2015**, 61, 306-314 | 5.1 | 1 |
| 312 | Characterization of multiferroic Bi0.8RE0.2FeO3 powders (RE=Nd3+, Eu3+) grown by the sol□el method. *Materials Letters*, **2015**, 139, 104-107 | 3.3 | 3 |

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| 311 | Thermoelectric and optoelectronic properties of a heterocyclic isoxazolone nucleus compound. *Materials Science in Semiconductor Processing*, **2015**, 30, 197-207 | 4.3 | 3 |
| 310 | Electronic properties of orthorhombic BaSn2S5 single crystal. *Indian Journal of Physics*, **2015**, 89, 437-443 | 1.4 | 1 |
| 309 | Structural, elastic, thermal and electronic properties of M2X (M = Sr, Ba and X = Si, Ge, Sn) compounds in anti-fluorite structure: first principle calculations. *Indian Journal of Physics*, **2015**, 89, 369-375 | 1.4 | 7 |
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