Publications

1. Peer reviewed International Journals (published/Communicated)

I. Chaurasiya, Rajneesh, Ambesh Dixit, and RavindraPandey. "Strain-mediated stability and electronic properties of WS2, Janus WSSe and WSe2 monolayers." ***Superlattices and Microstructures*** 122 (2018): 268-279.

II. Chaurasiya, Rajneesh, and Ambesh Dixit. "Defect engineered MoSSe Janus monolayer as a promising two dimensional material for NO2 and NO gas sensing." ***Applied Surface Science*** 490 (2019): 204-219.

III. Chaurasiya, Rajneesh, and Ambesh Dixit. "Ultrahigh sensitivity with excellent recovery time for NH 3 and NO 2 in pristine and defect mediated Janus WSSe onolayer." ***Physical Chemistry Chemical Physics*** (2020).

IV. Chaurasiya, Rajneesh, Goutam Kumar Gupta, and Ambesh Dixit. "Ultrathin Janus WSSe buffer layer for W (S/Se) 2 absorber based solar cells: A hybrid, DFT and macroscopic, simulation studies." ***Solar Energy Materials and Solar Cells*** 201 (2019): 110076.

V. Chaurasiya, Rajneesh Shubham Tyagi, Nirpendra Singh, SushilAuluck, and Ambesh Dixit, "Enhancing thermoelectric properties of Janus WSSe monolayer by inducing strain mediated valley degeneracy" ***Journal of Alloys and Compounds*** 855 (2021):157304.

VI. Chaurasiya, Rajneesh, Goutam Kumar Gupta, and Ambesh Dixit. "Efficient AZO/WSeTe/W(S/Se)2 heterostructures as efficient single junction solar cells with ultrathin Janus WSeTe buffer layer." ***." Journal of Physical Chemistry C*** (Under Review)

VII. Chaurasiya, Rajneesh, and Ambesh Dixit. "Current status and future possibility of low dimensional Janus transition metal dichalcogenides: Computational and Experimental Insight" (Manuscript under preparation)

2. Miscellaneous work

I. Sahu, Anurag, Rajneesh Chaurasiya, KirankumarHiremath, and Ambesh Dixit. "Nanostructured zinc titanate wide band gap semiconductor as a photoelectrode material for quantum dot sensitized solar cells**." *Solar Energy*** 163 (2018): 338-346.

II. Chaurasiya, Rajneesh, SushilAuluck, and Ambesh Dixit. "Cation modified A2 (Ba, Sr and Ca) ZnWO6 cubic double perovskites: A theoretical study." ***Computational Condensed Matter*** 14 (2018): 27-35.

III. Chaurasiya, Rajneesh, and Ambesh Dixit. "Point defects induced magnetism in CdO monolayer: A theoretical study." ***Journal of Magnetism and Magnetic Materials*** 469 (2019): 279-288.

IV. Gupta, Goutam Kumar, Rajneesh Chaurasiya, and Ambesh Dixit. "Dynamic stability and optoelectronic properties of Cu (Sb/Bi)(S/Se) 2 ternary chalcogenides: Promising ultrathin photoabsorber semiconductors**." *Solar Energy*** 177 (2019): 679-689.

V. Chaurasiya, Rajneesh, Ambesh Dixit, and RavindraPandey. "Strain-driven dynamic stability and electronic transitions in ZnX (X= O, S, Se, and Te) monolayers." ***Journal of Applied Physics*** 125, no. 8 (2019): 082540.

VI. Arumugam, S., P. Sivaprakash, Ambesh Dixit, Rajneesh Chaurasiya, L. Govindaraj, M. Sathiskumar, SouvikChatterjee, and R. Suryanarayanan. "Complex magnetic structure and magnetocapacitance response in a non-oxide NiF 2 system." ***Scientific reports*** 9, no. 1 (2019): 1-8.

VII. Gupta, Goutam Kumar, Rajneesh Chaurasiya, and Ambesh Dixit. "Theoretical studies on structural, electronic and optical properties of kesterite and stannite Cu2ZnGe (S/Se) 4 solar cell absorbers." ***Computational Condensed Matter*** 19 (2019): e00334.

VIII. Chaurasiya, Rajneesh, Radha Raman, Shubham Tyagi, and Ambesh Dixit. "Strain Modulated Optoelectronic Properties of CdO Monolayer." ***Journal of Electronic Materials*** 48, no. 6 (2019): 3963-3969.

IX. Dutta, Somrita, SudiptaSom, Mohan LalMeena, Rajneesh Chaurasiya, and Teng-Ming Chen. "Multisite-Occupancy-Driven Intense Narrow-Band Blue Emission from Sr5SiO4Cl6: Eu2+ Phosphor with Excellent Stability and Color Performance." *Inorganic Chemistry* 59, no. 3 (2020): 1928-1939.

X. Sakhuja, Neha, Ravindra Kumar Jha, Rajneesh Chaurasiya, Ambesh Dixit, and NavakantaBhat. "1T-Phase Titanium Disulfide Nanosheets for Sensing H2S and O2." ***ACS Applied Nano Materials*** 3, no. 4 (2020): 3382-3394.

XI. Kumar, Nilesh, Rajneesh Chaurasiya, and Ambesh Dixit. "Defects and light elements (Li, Be, B, C, O and F) driven d0 magnetism in InN monolayer" ***Vacuum*** *(2020): 109720.*