Research Collaboration Report: Dr. Dibya Prakash Rai, Assistant Professor, Department of Physics, Pachhunga University college, Aizawl, India

1. **Title:** Detrermining the promising properties of novel crystalline materials from density functional theory (DFT).

Collaboration Partners: On behalf of Dr. Tuan V Vu, Prof. Nguyen Thoi Truang, Director of Unstitute for Computational Science (INCOS) ton Duc Thang University (TDTU) Ho Chi Minh city, Vietnam and Dr. Amel Laref from Department of Physics, College of Science, King Saud University, Riyadh, Saudi Arabia.

Date of collaboration : 1st July 2018

The main objective of this research collaboration was to exchange ideas, sharing of knowledge, provide training in simulation to the young scholars. Also we are benefitted in utilizing the computational facilities (high-end-node cluster computers) for high level computational works. Under this collaborative work we have carriedout many research works and published these works jointly in many peer review, SCI, impact factor journals. The brief highlight of our work are as follows.

i. Electronic, Magnetic and Optical properties of monolayer (ML) hexagonal ZnSe on vacancy de-fects at Zn sites from DFT-1/2 approach. **D. P. Rai, A. Laref,** M. Khuili, S. Al-Qaisi, **T. V. Vu**, D. D. Vo, Vacuum, 182, 109597 (2020) [impact factor=4.11, SJR=Q1]

ii. Promising optoelectronic response of 2D monolayer MoS2: A first principles study. **D. P. Rai, T. V. Vu, A. Laref**, H. Joshi, P. K. Patra, Chemical Physics 538, 110824 (2020) [impact factor=2.55, SJR=Q2]

iii. Mechanical and thermodynamical properties of Fe2CoAl a full-Heusler alloy under hydrostatic pressure: A DFT study, H. Joshi, **T. V. Vu,** N. N. Hieu, R. Khenata, **D. P. Rai,** Materials Chemistry and Physics 270, 124792 (2021) [impact factor=4.778, SJR=Q2]

iv. Electronic, optical, and thermoelectric properties of Janus In-based monochalcogenides, **T. V. Vu,** V. T. T. Vi, H. V. Phuc, C. V. Nguyen, N. A. Poklonski, C. A. Duque, **D. P. Rai**, Journal of Physics: Condensed Matter 33 (22), 225503 (2021) [impact factor=2.75, SJR=Q2]

v. Theoretical prediction of electronic, transport, optical, and thermoelectric properties of Janus monolayers In2XO (X = S, Se, Te), Tuan V. Vu, Chuong V. Nguyen, Huynh V. Phuc, A. A. Lavrentyev, O. Y. Khyzhun, Nguyen V. Hieu, M. M. Obeid, D. P. Rai, Hien D. Tong, and Nguyen N. Hieu, PHYSICAL REVIEW B 103, 085422 (2021). [impact factor=3.908, SJR=Q1]

2. **Title:** Computational Material Science

Collaboration Partner: Prof. Mohan L. Verma, Head Department of Physics, Shri Shankarachary Technical Campus-SSGI, Bhilai, Chattishgarh, India.

Date of Collaboration: 1st February 2020.

In this collaboration we have discussed many critical phenomena of Computational Materials Science in relation to 2D energy materials for their potential application in future technology. I have also send my PhD scholar Mr. Bhanu Chettri to work in the computational lab of Prof. Verma for one month. During his stay he has learned SIESTA Code which is a density functional theory (DFT) based computational programing package. We also decided to share a joint supervisorship for guiding the PhD scholar and executing a joint research project, which is yet to formulate soon. Under this project we have published one research paper. Our findings include transition from non-magnetic semiconductor (pristine) → magnetic semiconductor (1C) → half-metal ferromagnetic (2C) → metal (3C) upon C-doping at N-site. In case of the B site, we observed metallic behaviour for 2C-doping. As 1,2 C-doping at the B site reduces the energy band gap from 1.8 eV to 0.81 eV, falls in the visible range and offers an opportunity to utilized as a photocatalyst material. C-doped systems show a magnetic semiconducting behavior crucial for spintronic applications.

i. Induced magnetic states upon electron–hole injection at B and N sites of hexagonal boron nitride bilayer: A density functional theory study, **B. Chettri**, P. K. Patra, S. Verma, B. K. Rao, **M. L. Verma**, V. Thakur, N. Kumar, **D. P. Rai,** International Journal of Quantum Chemistry 121 (16), e26680 (2021) [impact factor=2.44, SJR=Q2]

3. **Title:** The properties of sulvanite nanoparticles discuss in terms of theoretical methodology focused on the ab initio calculation

Collaboration Partners: Dr. Oksana Ismailova, Uzbek-Japan, Innovation Center of youth University Str. 2B, Tashkent city, 100095, Uzbekistan.

Date of Collaboration: 25th December 2020.

The main goal of this collaboration was to submit and execute an international Indo-Uzbek project. Our work is manily limited to analysis of physical properties based on the density functional theory by using various computational methods. Here we have collaborated with the experimental group from Uzbekistan to work on both experiment and theory. In this collaboration Dr. Lalhriatzuala, form Pachhunga University college and Prof. P. K. Patra from NEHU Shillong are also involved along with the Uzbek partners. With the help of this collaboration we could publish our work in ACS Omega. Herein we have presneted the results of family of ternary copper chalcogenides Cu3TaX4 (X = S, Se, and Te) from a*b initio* study. We report its potentiality in photovoltaic absorber materials in solar-cell devices. The electronic structure and optical properties are determined including electron–electron interaction and spin–orbit coupling (SOC), within the generalized gradient approximation plus Hubbard *U* (GGA+*U*) and GGA+*U*+SOC approximation. The large optical band gaps of Cu3TaS4 and Cu3TaSe4 considered ineffective for absorber materials, and also the hole effective mass has been modulated through applied pressure. These materials show extreme resistance to external pressure, and are found to be stable up to a pressure range of 10 GPa, investigated using phonon dispersion calculations. The observed optical properties and the

absorption coefficients within the visible-light spectrum make these compounds promising materials for photovoltaic applications.

i.Pressure-Induced Enhanced Optical Absorption in Sulvanite Compound Cu_3TaX_4 (X = S, Se, and Te): An *ab Initio* Study. H. Joshi, A. Shankar, N. Limbu, M. Ram, **A. Laref**, P. K. Patra, **O. B. Ismailova**, **D. P. Rai,** ACS omega 7 (23), 19070-19079 (2021) [impact factor=4.132, SJR=Q1]

4. **Title:** Study od the structural, electronic, piezoelectric and optical properties of materials

Collaboration Partner: Dr. Worasak Sukkabot, Department of Physics, Faculty of Science, Ubon Ratchathani University 85 Sathollmark Rd. Warinchamrab, Ubon Ratchthani, Thailand.

Date of Collaboration: 10th August 2021.

In collaboration with Dr. W. Sukkabot from Thailand, we could publish two research papers. Our collaborative work is mainly focus on the 2D hexagonal graphene like mtareials and 2D slab. We report the exchange and correlation electronic effect on the electronic and magnetic properties of transition metal mono- and co-doped 2D MoX_2 (X = S and Se) monolayers. The formation of the magnetism is caused by the double exchange mechanism, namely p-d and d-d hybridization. V, Cr and Co are the most energetically preferable substitutional dopants for these monolayers because of the lowest formation energies. Mn, Fe and Co doped-MoX_2 (X = S and Se) and (Mo, Co, Co) Se_2 monolayers are reflected as the half-metal behaviour with a perfect (100%) spin polarization at the Fermi level. Finally, the doped transition-metal dichalcogenide monolayers exhibiting the half metallic properties are hopefully proposed for the benefit of two-dimensional spintronic devices. In another work we performed the comparative study of the cubic bulk and its (001) surface of CsPbBr. The cubic bulk phase is mechanically stable compare to other bulk phases. We found the high optical spectra of absorption coefficient (10^7/cm) in the energy range of 3–6 eV for both the bulk and the surface favourable for opto-electronc applications.

i. Modulation of electronic and magnetic properties of MoX_2 (X= S and Se) monolayer via mono-and co-transition metal dopants: Spin density functional theory, W Thajitr, W Busayaporn, **D. P. Rai, W. Sukkabot,** Physica Scripta 97 (9), 095805 (2022) [impact factor=3.081, SJR=Q2]

ii. Electronic and optical properties of cubic bulk and ultrathin surface [001] slab of $CsPbBr_3$, H Joshi, RK Thapa, A Laref, **W. Sukkabot,** L Pachuau, L Vanchhawng, **D. P. Rai,** Surfaces and Interfaces 30, 101829 (2022)[impact factor=6.137, SJR=Q1]

(Prof. H.LALTHANZARA)

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