2D Materials and Electronic Devices Lab

Department of Physics
Harcourt Butler Technical University (HBTU) Kanpur

100 YEARS 1921 - 2021 Centenary Year

OBJECTIVE

- Atomistic Modeling of two-dimensional (2D) materials and its electronic devices using Density Functional Theory (DFT) Calculations.
- Study effect of Mechanical strain, external Electric Field and Twist angle on the electronic structure of 2D materials and its Heterostructure
- Doping enhancement in 2D Semiconductors
- Design and study Mixed-dimensional (0D/1D/2D/3D) materials based Heterostructure for various Optoelectronic and Energy applications.

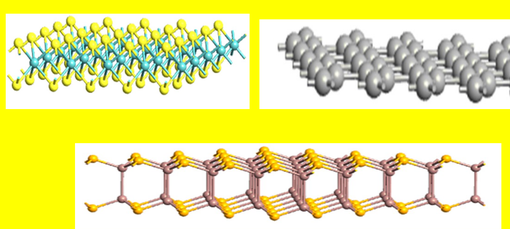
PRINCIPAL INVESTIGATOR

Dr. Divya Somvanshi (PI)

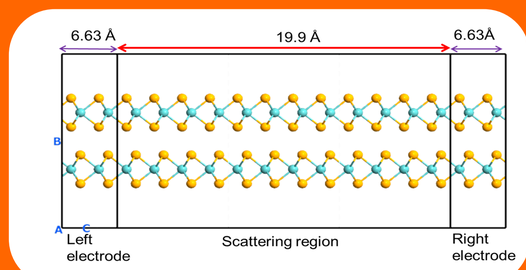
- PI is an Assistant Professor in the Department of Physics, School of Basic & Applied Sciences, HBTU, Kanpur.
- Ph.D. degree (Electronic Engineering) from IIT (BHU), Varanasi in 2015.
- Postdoctoral researcher from the IISc, Bangalore (June 2015-March 2016), Georgia State University, Atlanta, USA (Apr 2016- Aug 2017), and Technion-Israel Institute of Technology, Israel (March 2019-Feb 2020).
- DST INSPIRE Faculty at Jadavpur University, Kolkata India for the duration (Oct 2017-Feb 2019) to (March 2020-June 2022).

Research Focus

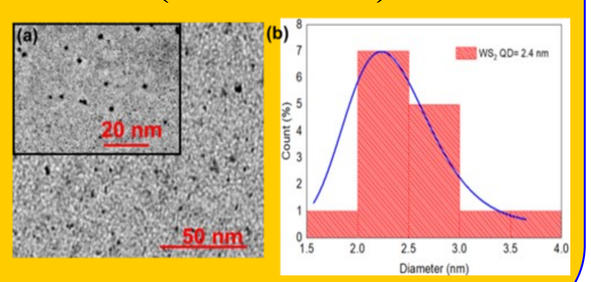
Atomistic Modelling of 2D Materials using DFT Calculations



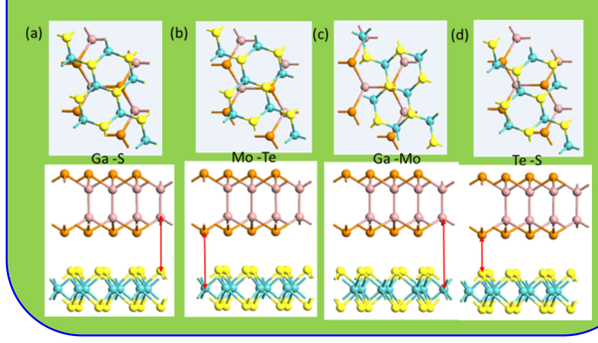
Electronic Transport in 2D Materials based Devices



Synthesis and Characterization of mixed-dimensional Material (2D/0D/1D/3D)



Twisting of 2D Materials and its Heterostructures

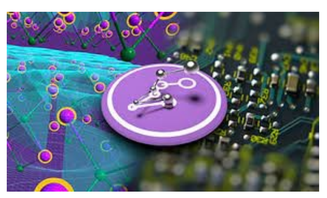


RESEARCH FACILITIES

⇒ Synapsis Quantum-Atomistic tool kit (ATK)

Quantum-ATK is an atomic-scale modeling software enables large -scale and more realistic material simulations, integrating multiple simulation methods, ranging from ab initio DFT to semi-empirical and classical force

SYNOPSYS® QUANTUMATK



⇒ High Performing Computation –

- All in one Desktop (AIO) -2 HP-workstation Z2G8: Intel-i7-11700/16 GB/1TB SATA harddrive disk, 2021
- HP IDS ProOne 400 G5 20 inch HD+ Non-Touch All-in-One Business PC. 2020.
- HP ProOne 400 G3 20 inch Non-Touch All-in-One intel Core i5

RESEARCH OUTCOME

- S. Chowdhury, A. Mishra, P. Venkateswaran, **Divya Somvanshi,** Electronic structure and optical properties of GaTe/$MoTe_2$ based vdW heterostructure under mechanical strain and external electric fields, *Materials Science in Semiconducting Processing*, Vol. 163, 15 August 2023, 107572 (I.F = 4.67)
- S. Chowdhury, P. Venkateswaran, **Divya Somvanshi**, Strain-dependent doping and optical absorption in Al-doped graphene-like ZnO monolayer, *Solid State Communications*, 365, 115139, 2023. (I.F: 1.93)
- S. Chowdhury, P. Venkateswaran, **Divya Somvanshi**, "Biaxial strain tuning of the electronic and optical properties of Nb, Ta and Re-doped WSe2 monolayer: a first-principles study", *Physica B: Condensed Matter*, Vol 653, 414668, 2023, (I.F. 2.98)
- S. Chowdhury, P. Venkateswaran, **Divya Somvanshi**, "Interlayer twist angle-dependent electronic structure and optical properties of InSe/WTe_2 van der Waals heterostructure", IEEE International Conference of Electron Devices Society Kolkata (EDKCON), India, 26-27 November 2022, Pages: 325-328, 2022
- S. Chowdhury, P. Venkateswaran, **Divya Somvanshi**, Strain-Induced Electronic Structure and Bandgap Transition in Bilayer of AB and AA Stacking Order, 2022 IEEE Calcutta Conference (CALCON), Kolkata, India, 10-11 Dec, 2022, IEEE Conference Proceeding, Pages: 191-195, 2022

COLLABORATION

Prof. Satyabrata Jit, IIT(BHU), Varanasi
Prof. P. Venkateswaran, Jadavpur University (JU), Kolkata
Prof. A. G. U. Perera, Georgia State University (GSU), Atlanta USA

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