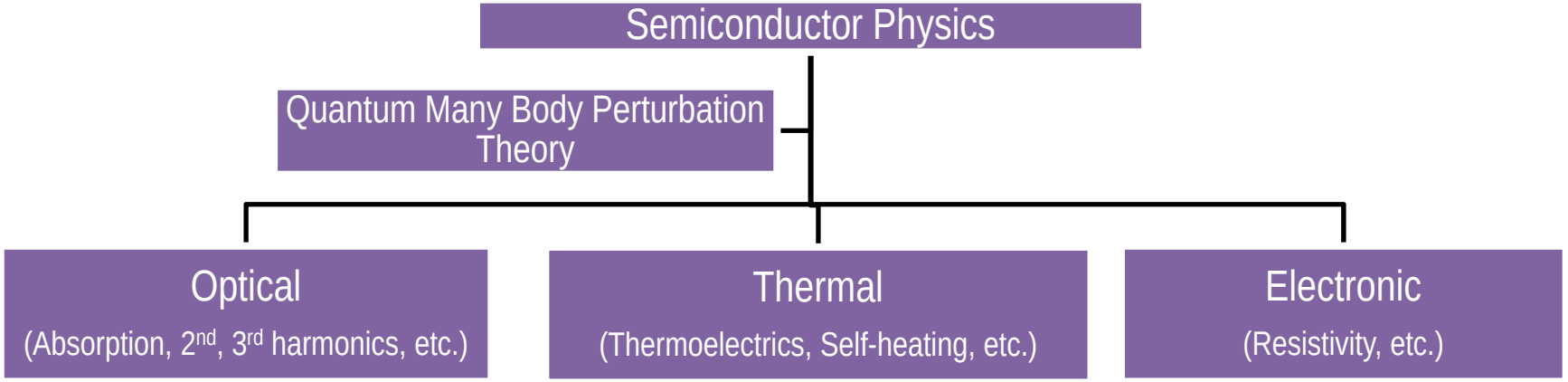
Electronic Structure Group Theory

Group leader:
Sitangshu Bhattacharya,
Assistant Professor,
Department of Electronics and Communication Engineering,
Indian Institute of Information Technology- Allahabad,
Email: sitangshu@iiita.ac.in

Research Activities : Ab-initio Electronic Structure Theory Calculations



Selected Publications:

Himani Mishra and Sitangshu Bhattacharya, Phys. Rev. B, 99 165201 (2019).
Himani Mishra, Anindya Bose, Amit Dhar and Sitangshu Bhattacharya, Phys. Rev. B, 98 045138 (2018).

Research Activities : Ab-initio Electronic Structure Theory

Materials: III-V (GaAs, InAs, etc.), TMDCs (WSe_2, MoS_2, etc.), etc.

Methods:

First principles calculations: All branches: DFT, RPA, TD-DFT, GW, Screen-Exchange (SEX)
Electron-phonon self energy calculations
Static and real-time Bethe-Salpeter Equation
Modern theory of time-dependent electric polarization in materials
Lattice anharmonic effects

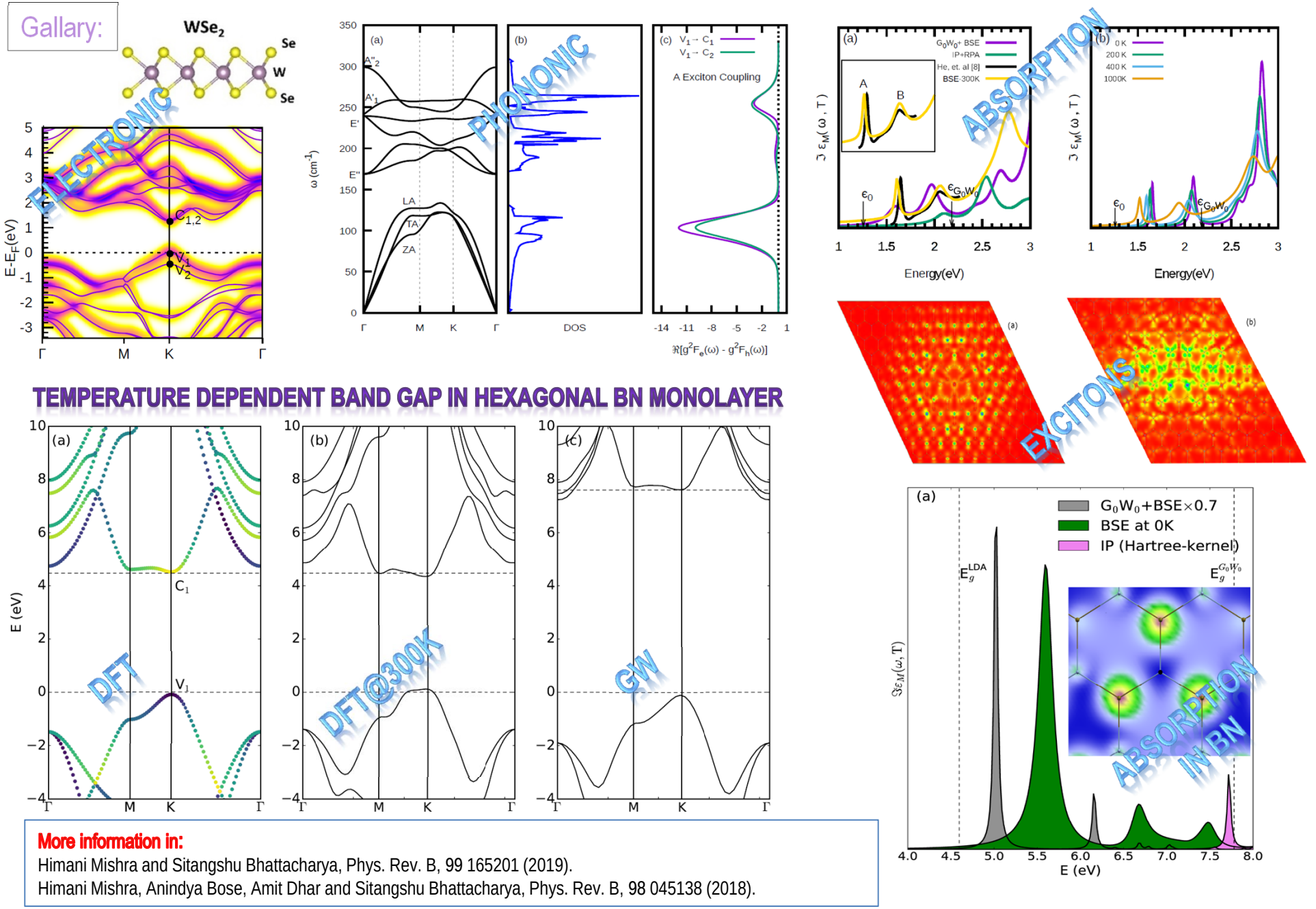
Resources: High performance computational (HPC) facility having 16 computational nodes with a total 640 cores 5.9 TB of RAM connected to a storage capacity of 450 TB with a data transfer rate of 100 Gbps. Apart from this we also have 4 GPU nodes each having two NVIDIA TESLA V-100 with 16 GB of RAM. The facility is exclusively dedicated to carry out calculations using licensed packages of Vienna Ab initio Simulation Package (VASP), Quantum Espresso and Yambo.

Results:

Electronic and phononic: Band structures, interaction strength, etc.
Thermal properties: Bulk modulus, thermal expansion, conductivity, elasticity, etc.
Ultrafast spectroscopy: Absorption spectra, optical transitions, exciton lifetime, 2^{nd}, 3^{rd} harmonic generations, optical frequency conversions and mixings

Research Activities : Ab-initio Electronic Structure Theory

Gallary:



More information in:

Himani Mishra and Sitangshu Bhattacharya, Phys. Rev. B, 99 165201 (2019).

Himani Mishra, Anindya Bose, Amit Dhar and Sitangshu Bhattacharya, Phys. Rev. B, 98 045138 (2018).