RESEARCH

(i) Formulation of a New Exchange-Correlation Potential Functional for Better Band Gaps in Density Functional Theory (DFT) – Completed (To be published)

(ii) Effect of Strain Engineering on the Band Gap, Fermi Energy and the Carrier Effective Mass of GaX (X= P, N, As, Sb, and Bi) – Completed (To be published)

(iii) Doping-Induced Indirect-Direct Band Gap Transition of Silicon – completed (Submitted for Publication)

(iv) Atomistic Simulation of Metal-ion Batteries using Ab Initio Data – In progress

(v) First Principle Investigation of Thermoelectric Properties of $Bi2(S_1\text{-}xTe_x)_3$ via Density Functional Theory (DFT) – In progress

(vi) Investigation of Strain Engineering Effect on the electronic and Mechanical Properties of Cadmium Telluride via Density Functional Theory (DFT) – In progress

(vii) Discovery of Seven New MgCrF5 Cathode Materials for Magnesium-Ion Batteries (Submitted for publication)