School of Nano Science

School of PHYSICS

IPM Condensed Matter & Statistical Physics Group

Weekly Seminar

Effective deformation potentials of phosphorene: an ab-initio study

Invited speaker:

Dr. Mohammad Elahi

Post Doctoral Researcher at the School of Electrical and Computer Engineering, University of Tehran

Abstract:

Electron-phonon interaction in single-layer phosphorene is studied from first principles based on the density functional theory, using finite displacement method. Scattering rates are numerically evaluated for carriers in the conduction and valence bands. A criterion for the selection of phonon wave-vector in scatterings is proposed. Scattering selection rules are studied, utilizing group theory for the structure with $D_{2 h}^7$ space group symmetry. Approximate analytical formulas for scattering rates, adopting the anisotropy intrinsic to phosphorene, are derived, and effective deformation potential are extracted by fitting the formulas to numerical scattering rates extracted from ab initio calculations.

Wednesday, 29th of Day(1395) (January 18th, 2017), 14:00-15:00

Farmaniyeh seminar room