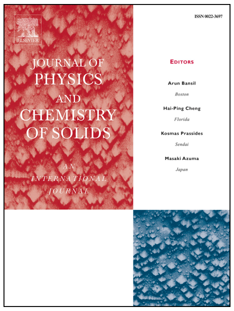

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Optical Properties of graphene, silicene, germanene, and stanene from IR to far UV – A First Principles Study

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ABSTRACT

This study offers an analysis of optical properties of Graphene and its 2D analogues: Silicene, Germanene, and Stanene with the help of band structures based on Density Functional Theory. The complex dielectric function and complex refractive index are calculated in both parallel (||) and perpendicular (⊥) polarization directions of the electromagnetic field. From these calculated values, optical observables like absorption, reflection, optical conductivity, and electron loss function have been studied. The optical response of all materials is shifted from ultraviolet (UV) to infrared (IR) from graphene to stanene; Graphene is more into UV region and other materials in the IR and visible regions. The intensity of absorption is maximum for stanene. The real part of dielectric function reveals the existence of plasma frequency in the || polarization direction indicating the metal to dielectric transition except for graphene. Study on refractive index clearly displays the birefringence characteristics of all materials. Reflectivity is enhanced in the mid IR and visible regions when light is polarized in the || direction. The in-depth investigations arrive at fine results which would enable the prediction of their potential applications in the optical and optoelectronic industries.

Keywords: 2D materials, graphene, silicene, germanene, stanene, optical properties

1. Introduction

The exotic properties exhibited by graphene, leads to the further exploration of its 2D counterparts: silicene, germanene, and stanene. Though these materials exhibit extraordinary properties due to the presence of linearity at the Dirac point they are refrained from its applications in the semiconductor and optical industry due to their gapless electronic dispersion [1-7]. However the structural differences due to the presence of buckling in silicene, germanene, and stanene provides an added advantage for them to be integrated with substrates [8], [9], [10]. Moreover, each material is found to have its own significant property. Unlike graphene, the band gap is controllable in silicene with transverse external static electric field [11] ,[12]. The intrinsic carrier mobility in germanene is predicted to be higher than silicene due to the weak coupling of charge carriers with in-plane phonons and the large buckling of germanene [13]. Tin being the heaviest element in the group is expected to have enhanced spin-orbit coupling that facilitates stanene to possess outstanding properties: room temperature topological insulator effects [14], increased thermoelectricity