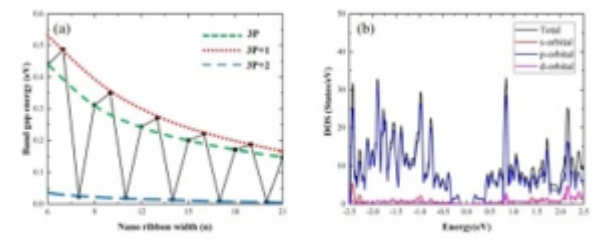
Our new paper in Physica E: Low-dimensional Systems and Nanostructures

Congratulations for the publication of paper “The electronic and optical properties of armchair germanene nanoribbons”

By Arash Karaei Shiraz, Arash Yazdanpanah Goharrizi, Seyedeh Mehri hamidi

The electronic and optical properties of armchair germanene nanoribbons (AGeNRs) are studied using the first principles calculations. The band structure, band-gap size, projected density of states (PDOS), and dielectric function of AGeNRs are calculated. Moreover, the variation of these parameters as a function of various ribbon widths is investigated. By increasing the width of ribbons the band-gap size of pristine AGeNRs is decreased according to three different trends. Based on these trends, it is extracted that the AGeNRs can be divided into three categories named as n=3P, n=3P+1, n=3P+2, here n is the number of germanium atoms in the width and P is an integer. Moreover, all these categories are direct band-gap materials and the order of band-gap size is changed as: $E_G(3P+2) < E_G(3P) < E_G(3P+1)$. Due to the direct band-gap size, it can be extracted that all of AGeNR categories are proper for optical applications. Based on the simulation results of this work, it is demonstrated that the AGeNRs are appropriate for optical devices in the range of infrared applications. In addition, the effect of uniaxial tensile and compressive strain on the band-gap size and the dielectric function of AGeNRs is investigated and it is shown that the electronic and optical properties of AGeNRs can be tuned by strain in a wide range.


(a)
3P
3P+1
3P+2
Band gap energy (eV)
Nano ribbon width (n)
(b)
Total
s-orbital
p-orbital
d-orbital
DOS (States/eV)
Energy(eV)