عنوان مقاله:

Theoretical study of sodium doped blue phosphorene nanotubes

محل انتشار:

اولین کنفرانس ملی نانو از سنتز تا صنعت (سال: 1396)

تعداد صفحات اصل مقاله: 1

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خلاصه مقاله:

Introduction: Similar to graphene, blue phosphorene has a honeycomb-like structure, but it is non-planar [1]. What distinguishes phosphorene from other 2D materials is its anisotropic structure, which leads to direction-dependent electronic properties [2,3].Method: The geometry relaxation and electronic structure calculations were performed using linear combination of atomic orbitals (LCAO) as implemented in the SIESTA package. The exchange-correlation functional of the electrons was described by the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE). An energy cutoff of 180 Ry was chosen and the Brillouin zone k-point sampling was set 1×1×10 for all the nanotubes, based on the Monkhorst-Pack method. The nanotubes were relaxed until the residual forces on each atom were reached below 0.01 eV/Å.Results and conclusion: The first-principle calculations reveal that blue phosphorene nanotubes are semiconductors with indirect band gap and by increasing the diameter of the nanotubes, the band gap increases. In addition, the effect of doping with sodium atom on the structural and electronic properties of these nanotubes were studied. According to the obtained results, total energy of phosphorene nanotubes .decreases by entring sodium atom, so the chemical stability increases

کلمات کلیدی:

Blue Phosphorene Nanotubes, Sodium Atom, Density Functional Theory