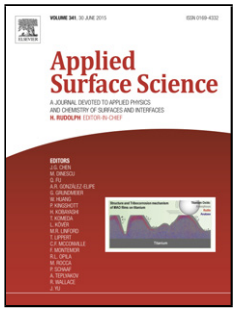

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Electronic properties of graphene with single vacancy and Stone-Wales defects

Esmaeil Zaminpayma[1], Mohsen Emami Razavi[2], Payman Nayebi [3]

[1] Physics Group, Qazvin Branch, Islamic Azad University, Qazvin, Iran

[2] Plasma Physics Research Center, Science and Research Branch, Islamic Azad University, P.O. Box 14665-678, Tehran, Iran

[3] Department of physics, College of technical and engineering, Saveh branch, Islamic Azad University, Saveh, Iran

Highlights

- The first principles calculations have been performed based on self-consistent charge density functional tight-binding in order to examine the electronic properties of graphene device with single vacancy (SV) and Stone-Wales (SW) defects.
- We have studied the density of state, current voltage curves and transmission spectrum of pristine graphene and graphene with single vacancy (SV) and Stone-Wales (SW) defects.

Abstract

The first principles calculations have been performed based on self-consistent charge density functional tight-binding in order to examine the electronic properties of graphene with single vacancy (SV) and Stone-Wales (SW) defects. We have optimized structures of pristine graphene and graphene with SV and SW defects. The bond lengths, current-voltage curve and transmission probability have been calculated. We found that the bond length for relaxed graphene is 1.43 Å while for graphene with SV and SW defects the bond lengths are 1.41 Å and 1.33 Å, respectively. For the SV defect, the arrangement of atoms with three nearest neighbors indicates sp_2 bonding. While for SW defect, the arrangement of atoms suggests nearly sp bonding. From the current-voltage curve for graphene with defects we have determined that the behavior of the I−V curves is nonlinear. It is also found that the SV and