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Effect of vacancy in penta-graphene nanoribbons: Afirst principals study KHALDOUN TARAWNEH, Princess Sumaya University for Technology, NABIL AL-AQTASH, Hashemite University, RENAT SABIRIANOV, University of Nebraska at Omaha — Penta-graphene has been proposed recently as a new stable carbon alltrope which is stronger than graphene. To farther explore its properties, we use the first-principals calculations to reveal that the electronic properties of penta-graphene nanoribbons can be modified in the presence of vacancy defect. Our calculations showed that the band gap of penta-graphene nanoribbons changes with changing the width of the ribbons and on the position of the vacancy relative to its edge. The vacancy formation energy is calculated to be 8.42 eV in the middle of the ribbons and decreases to 6.8 eV when the vacancy position is close to the edge of the ribbon. These results for a stable nanoribbon with a large band gap is promising for designing optoelectronic devices.

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