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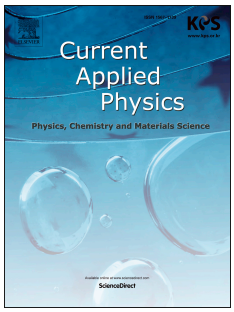

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PII: S1567-1739(18)30204-9

DOI: 10.1016/j.cap.2018.07.014

Reference: CAP 4796

To appear in: *Current Applied Physics*

Received Date: 7 May 2018

Revised Date: 8 July 2018

Accepted Date: 15 July 2018

Please cite this article as: M. Mirakhory, M.M. Khatibi, S. Sadeghzadeh, Vibration analysis of defected and pristine triangular single-layer graphene nanosheets, *Current Applied Physics* (2018), doi: 10.1016/j.cap.2018.07.014.

Vibration analysis of defected and pristine triangular single-layer graphene nanosheets

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Abstract

This paper investigates the vibration behavior of pristine and defected triangular graphene sheets; which has recently attracted the attention of researchers and compare these two types in natural frequencies and sensitivity. Here, the molecular dynamics method has been employed to establish a virtual laboratory for this purpose. After measuring the different parameters obtained by the molecular dynamics approach, these data have been analyzed by using the frequency domain decomposition (FDD) method, and the dominant frequencies and mode shapes of the system have been extracted. By analyzing the vibration behaviors of pristine triangular graphene sheets in four cases (right angle of 45-90-45 configuration, right angle of 60-90-30 configuration, equilateral triangle and isosceles triangle), it has been demonstrated that the natural frequencies of these sheets are higher than the natural frequency of a square sheet, with the same number of atoms, by a minimum of 7.6% and maximum of 26.6%. Therefore, for increasing the resonance range of sensors based on 2D materials, non-rectangular structures, and especially the triangular structure, can be considered as viable candidates. Although the pristine and defective equilateral triangular sheets have the highest values of resonance, the sensitivity of defective (45,90,45) triangular sheet is more than other configurations and then, defective (45,90,45) sheet is the worst choice for sensor applications.

Keywords: Resonance; Pristine and defected Triangular sheet; Graphene; Molecular dynamics; Frequency domain decomposition