## عنوان مقاله:

Fracture Analysis of Vacancy Defected Nitrogen Doped Graphene Sheets Via MD Simulations

## محل انتشار:

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## خلاصه مقاله:

The novel hexagonal monolayer sheet of carbon atoms, graphene, has attracted great attention due to their exceptional electrical and mechanical properties. Their phenomenally high strength and elastic strain, nevertheless, can be altered by structural defects due to stress concentration. In this paper, the fracture behaviour of graphene sheets and nitrogen doped graphene sheets with vacancies were investigated using molecular dynamics (MD) simulations at the different temperatures of ۳۰۰K, ۵۰۰K, and ۹۰۰K. The results reveal a significant strength loss caused by both the defects and vacancies and doped nitrogen in graphene. The deformation process of graphene at various strain rate levels, with regard to the failure behaviour, is discussed. The validity of the proposed MD simulations is verified by comparing the simulation results with the available predictions from the quantized fracture mechanics.

## کلمات کلیدی:

Graphene, Defect, Fracture analysis, Nitrogen doped graphene, Molecular dynamics simulations