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Structural, stability and vacancy properties of both defect free and defected 2D h-BNNSs.

The structural, stability and vacancies properties of both defect free and defected 2D h-BNNSs were studied using the classical molecular dynamics (MD) approach. The calculations were performed in the NVT Evans and NPT hoover ensembles using the Tersoff potentials with the Verlet leapfrog algorithm to obtain reliable structural properties and energies for defect free, boron (B) and nitrogen (N) vacancies. B and N defect energies were calculated relative to the bulk defect free total energies, and the results suggest that N vacancy is the most stable vacancy as compared to the B vacancy. The radial distribution functions and structure factors were used to predict the most probable structural form. Mean square displacements suggests the mobility of B and N atoms in the system, which is increasing with an increase in the surface area of the nanosheets. Results obtained are compared with the bulk defect free h-BNNSs.

Apply to be considered for a student ; award (Yes / No)?

yes

Level for award;(Hons, MSc, PhD, N/A)?

MSc

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