Monatomic reactions with single vacancy monolayer h-BN: DFT studies†

ABSTRACT

Hexagonal boron nitride (h-BN) has been widely utilized in various strategic applications. Fine-tuning properties of BN towards the desired application often involves ad-atom adsorption of modifying its geometries through creating surface defects. This work utilizes accurate DFT computations to investigate adsorption of selected 1st and 2nd row elements (H, Li, C, O, Al, Si, P, S) of the periodic table on various structural geometries of BN. The underlying aim is to assess the change in key electronic properties upon the adsorption process. In addition to the pristine BN, B and N vacancies were comprehensively considered and a large array of properties (i.e., atomic charges, adsorption energies, density of states) were computed and contrasted among the eight elements. For instance, we found that the band gap to vary between 0.33 eV (in case of Li) and 4.14 eV (in case of P). Likewise, we have illustrated that magnetic contribution to differ substantially depending on the adatom adsorbents. Results from this work has also lays a theoretical foundation for the use of decorated and defected BN as a chemical sensor for CO gases