

Energy decomposition analysis of 2D boron crystals from first principles

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Very recently, a monolayer boron crystal has been successfully grown on the Ag(111) surface under ultrahigh vacuum [1]. The structure of that crystal can be described as an arrangement of boron atoms on a hexagonal (triangular) lattice with some fraction of atoms missing. The distribution of the missing atoms (vacancy sites in the triangular lattice) depends on many factors, and one of them is the amount of charge that is transferring from the substrate to the 2D crystal. Furthermore, an uncharged freestanding crystal, which is known in the literature as the α -sheet [2], has evenly distributed vacancies as it is shown in Fig. 1.

The purpose of this investigation is to decompose the total energy of a 2D boron crystal into energy contributions coming from the constituent atoms according to their coordination number. We may write:

$$E_{tot}(n_3, n_4, n_5, n_6, q) = \frac{1}{N} \sum_{i=3}^6 n_i e_i^q$$

where n_i and e_i^q are the number of boron atoms in the unit cell with i nearest neighbours and their energy, respectively. N is the total number of atoms per unit cell. The individual energy contributions, e_i^q , are found from separate first principles computations for 2D boron crystals in which each atom has i nearest neighbours. One example is the boron graphitic structure from which we calculate e_3^q . We show that by using such a simple energy decomposition it is possible to predict, with reasonable accuracy, the total energy of any 2D boron crystal (with any particular distribution of vacancy sites). Furthermore, the model is extendable to charged structures (with charge q), for which we calculate, from first principles, an appropriate set (e_i^q) of energy values.

For instance the estimated binding energy, $E_b = E(\text{isolated B atom}) - E_{tot}(n_i, q)$, for the uncharged α -sheet is 6.55 eV, which differs by only 50 meV from the 'true' 6.6 eV value calculated using first principles computations. We also show that in contrast to neutral structures that give preference to coordination number 5, in negatively charged structures the atoms prefer to be 3- and 4-coordinated. A detailed comparison with experimental results will be presented.

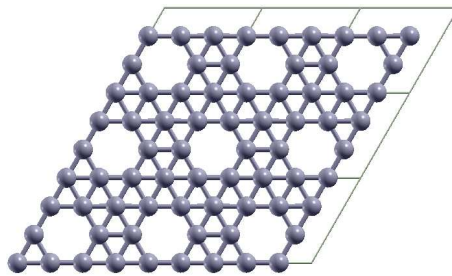


Figure 1: Structure of the α boron sheet.

[1] A. J. Mannix et al., *Science* **350**, 1513 (2015).

[2] H. Tang and S. Ismail-Beigi, *Phys. Rev. Lett.* **99**, 115501 (2001).