A single boron sheet is considered as a new nanomaterial with promising applications in electronics and as a sensor device. In this study we present quantum-mechanical molecular dynamic (QCMD) calculation of reflection, adsorption, and transmission processes of hydrogen impacting at energy range 0.25 to 100 eV on a single boron sheet and electron transport study through the system. Quantum-mechanical component of our QCMD approach is self-consistent charge tight binding density functional theory method (SCC-DFTB). We have considered the corrugated boron sheet as our target, created experimentally [2], and compare our results with those reported for graphene [3], showing noticeable differences. Also, we utilized the open boundary non-equilibrium Greens function method to obtain conductivity of borophene as a function of hydrogen coverage. Our results suggest that borophene has favorable properties for its use as a hydrogen detector.

**Abstract**

**DFT-PAW method**
- We have benchmarked our DFTB pair-potentials with the DFT-PAW method implemented in the Vienna ab-initio simulation package (VASP) [4,5].
- The calculations were carried out in a fully periodic system where the Kohn-Sham equations have been solved variationally in a plane wave basis set using the projector-augmented-wave (PAW) method of Blochl [6], as adapted by Kresse and Joubert [7].
- We have chosen the functional of Perdew, Burke, and Emzerhof (PBE) [8] based on the generalized gradient approximation.
- The benchmarks were carried out in both methods, as a series of static calculations of the approach of a Hydrogen atom to different adsorption sites on the borophene and graphene sheet.
- A Monkhorst-Pack k-point mesh of 16x1x1 was used in both DFT and DFTB calculations.
- The kinetic energy cutoff for the VASP plane wave basis was set to 400 eV.

**RESULTS: DFT and SCC-DFTB comparison**
- The potential energy curves of different hydrogen adsorption sites for a-c) borophene and d) graphene. SCC-DFTB overestimates the bonding energies for different hydrogen adsorption sites. Typical difference of the potential barrier is 0.05 eV/atom with respect to the DFT results. This validates our SCC-DFTB approach.

**Conductance of borophene by NEGF**


**DFTB comparison**

- Quantum Classical Molecular Dynamics is used to model hydrogen irradiation on a quasi-planar boron sheet by the self-consistent-charge density functional tight binding approach.
- The charge dynamics are treated by DFTB, based on a second order expansion of the Kohn-Sham total-energy functional [1] with density integral parametrized and predefined Hamiltonian and overlap integrals, and repulsive potentials are fitted by splines to the system Slater-Koster parameters [2].
- We prepare an infinite corrugated boron sheet with a target of 1nm² with semi-periodic boundary conditions which is energy optimized and thermalized to 300 K prior to the bombardment with hydrogen atoms in 0.25-100 eV impact energy range.
- The collision dynamics are done by the velocity Verlet algorithm and the projectile velocity is parallel to the surface normal at a time step of 0.25 fs, which lasts 300-500 fs.
- We used a series of 2000 samples in which the initial position of the hydrogen atom was homogeneously distributed at a distance of 0.7 nm from the upmost boron layer.

**Conclusions**

- Potential energy curves obtained by DFT and SCC-DFTB are in good agreement.
- Boron sheet can capture on average more hydrogen atoms at 2-10 eV, where graphene only reflects and transmits them.
- The boron sheet has a maximum reflection of 20% at 5 eV while graphene has maximal reflection at 2 eV. This difference shows that a boron based device would suffer a lower loss of detection compared to a graphene based device.
- The angular distribution of reflected H atoms shows that at lower energies (0.25-5 eV) no absorption.
- The conductance in x-direction decreases about 8 times when hydrogen atoms two sided coverage increases from virgin borophene to full coverage, illustrating that borophene as an effective hydrogen detector.

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**References**