Supplementary Material

(Dated: July 3, 2022)

I. METHODS

We evaluate the binding energies with vdW-DRSSL functional and apply a correction for basis set superposition error (BSSE)[1]. The BSSE refers to the overestimation of binding energy when comparing the total energy of a combined system and its components obtained from simulations with localized basis sets. This overestimation is a consequence of additional orbitals at the interface, which can be shared between the two components to lower their individual energy. To correct this error we calculate the total energy of the components using ghost orbital, i.e. basis set functions without associated electrons. The corrected binding energy is given

$$E_{Binding} = E(\text{bismuthene} + \textit{subs.}) - E(\text{bismuthene} + \textit{ghost}\ \text{subs.}) - E(\textit{ghost}\ \text{bismuthene} + \text{subs.}) \quad (1)$$

II. ADDITIONAL RESULTS

A. Surface terminations of SiO_2

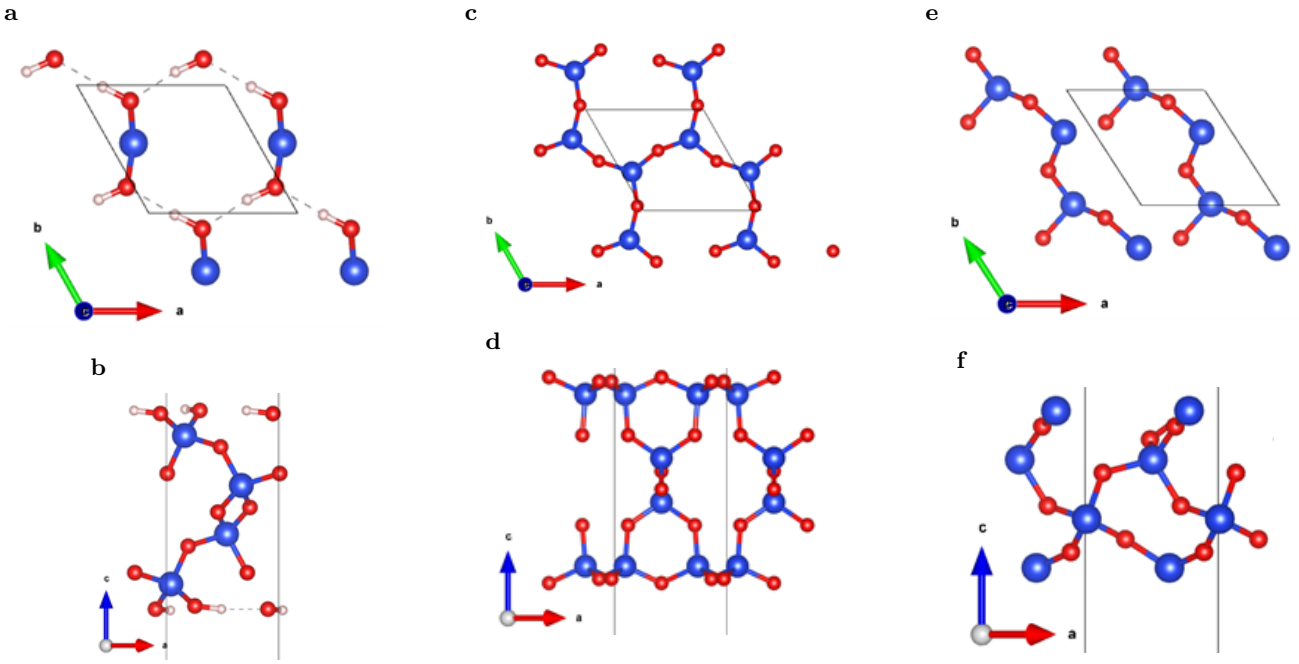

FIG. 1. Crystal structure of **SiO_2 slabs** with different surfaces in side (a,c,e) and top view (b,d,f): hydroxylated (OHT) (a,b), reconstructed oxygen terminated (ROT) (c,d), and silicon terminated (SiT) (e,f); in side view (a,c,e) and top view (b,d,f)

B. Flat-hexagonal bismuthene@ROT-SiO_2

The f-hex@ROT-SiO_2 heterostructures consist of one f-hex unit cell and one substrate cell with -4% strain, while f-hex@SiT-SiO_2 and f-hex@SiT-SiO_2 consist of $(\sqrt{3}\times\sqrt{3})$R30° b-hex supercell on top of a 2×2 substrate supercell with 5% strain.

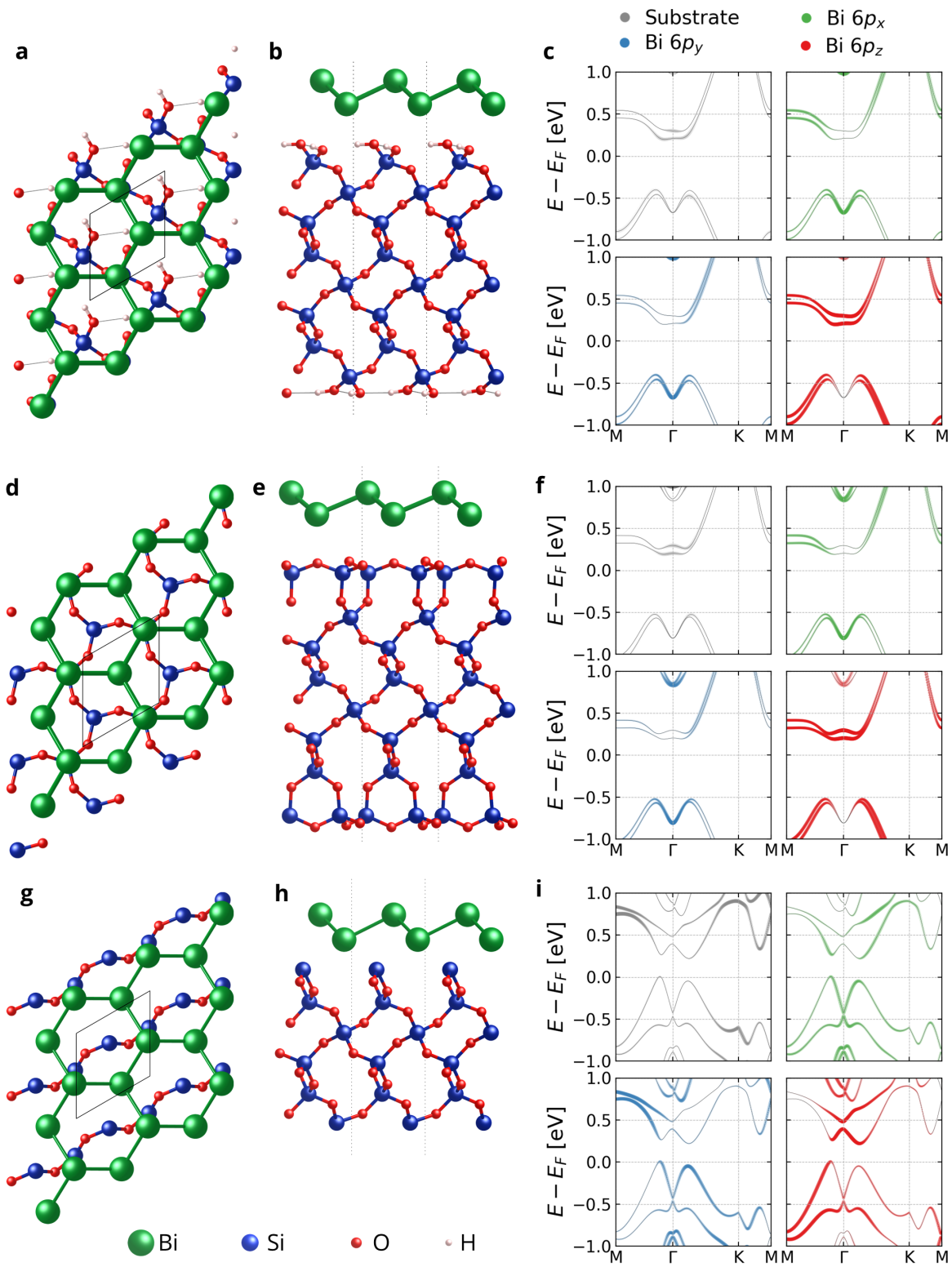

FIG. 2. Crystal structure of flat hexagonal bismuthene on SiO_2 (top view and side view) and orbital projected DFT electronic band structure for three different surface terminations: hydroxylated (**a-c**), reconstructed (**d-f**), and Si terminated (**g-i**). In each panel the contribution of different orbitals is proportional to the line width. Bi 6*s* orbitals do not contribute to the bands near the Fermi level.

C. Strain effect in buckled-hexagonal bismuthene

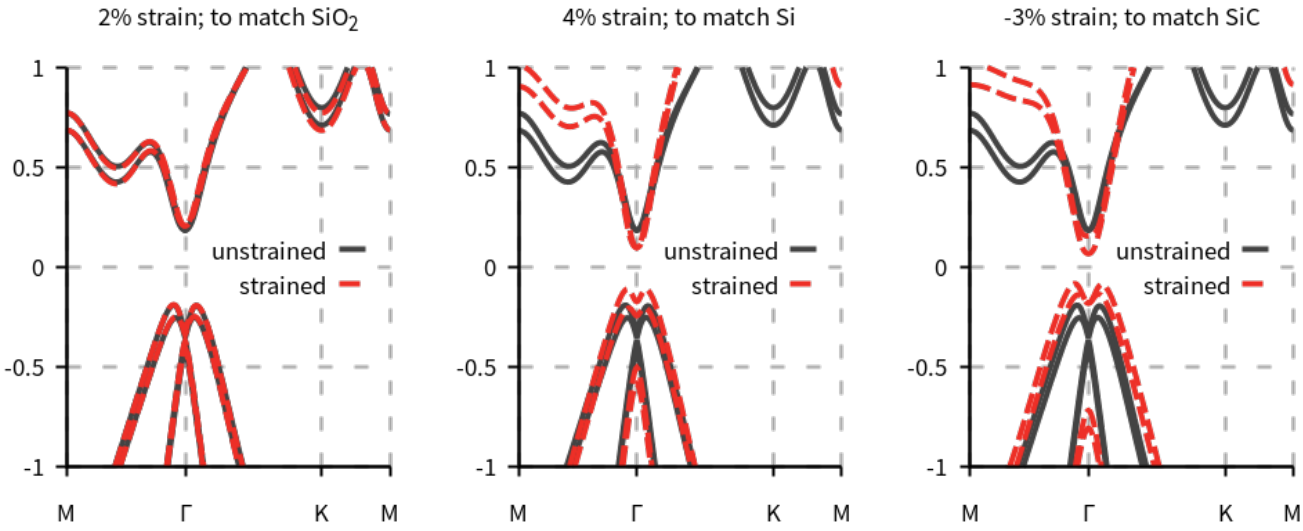

FIG. 3. Effect of the strain on the band structure of free-standing b-hex bismuthene. The topological features are resilient to strain.

[1] S. Boys and F. Bernardi, Molecular Physics **19**, 553 (1970).