Tuning the Topological Band Gap of Bismuthene with Silicon-based Substrates

Nils Wittemeier[1]
Pablo Ordejón[1] and Zeila Zanolli[2]
[1]*Catalan Institute of Nanoscience and Nanotechnology - ICN2 (CSIC-BIST), 08193 Barcelona, Spain*
[2]*Chemistry Department and, Debye Institute for Nanomaterials Science, Utrecht University, 3508 TA Utrecht, The Netherlands*
nils.wittemeier@icn2.cat

Bismuth plays a crucial role in many compounds with Topological Insulator [1] properties due to its strong intrinsic spin-orbit interaction. Some meta-stable polymorphs of bismuth monolayer (bismuthene) can host topologically nontrivial phases. [2, 3] However, it remains unclear if these polymorphs can become stable through interaction with a substrate, and, in that case, whether their topological properties are preserved, and how to design an optimal substrate to make the topological phase more robust.

To answer these questions, we performed a comprehensive DFT study of the interactions between bismuthene and silicon-based substrates. [4] We demonstrate that bismuthene polymorphs can become stable over silicon carbide (SiC), silicon (Si), silicon dioxide (SiO2) and that the proximity interaction in the heterostructures has a significant effect on the electronic structure of the monolayer, even when bonding is weak. We further show that the van der Waals interactions and the breaking of the sublattice symmetry are the main factors driving changes in the electronic structure. Our work demonstrates that substrate interaction can strengthen the topological properties of bismuthene polymorphs and make them accessible for experimental investigation and technological applications.

References

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Figures

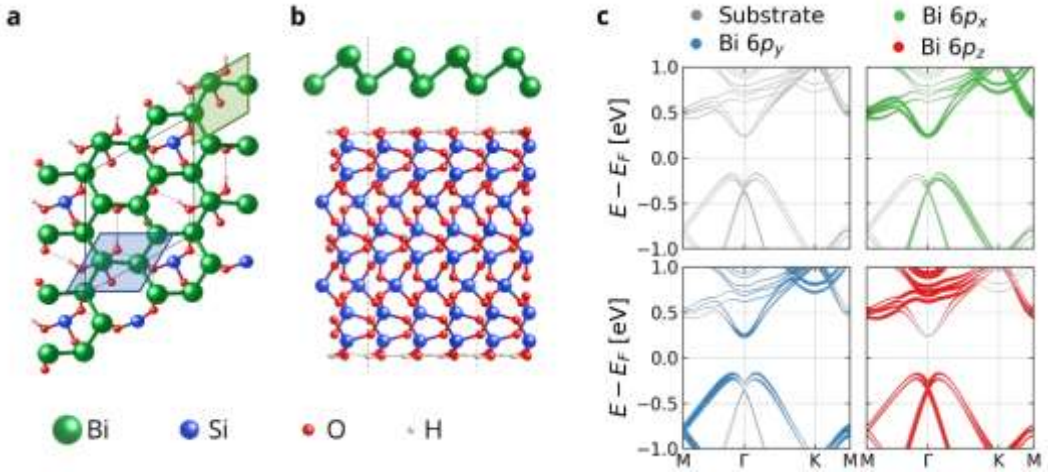

Figure 1: Crystal structure of buckled hexagonal bismuthene on hydroxylated SiO_2 ((a) top and (b) side views) and orbital projected band structure (c). Signature of band inversion is visible in the projection of Bi $6p_y$ orbitals.