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Interfaces between buckling phases in Silicene MATHEUS P. LIMA, ANTÔNIO J.R. DA SILVA, ADALBERTO FAZZIO, University of São Paulo — Silicene has a honeycomb buckled lattice, with two energetically degenerate geometric phases (α and β). The α phase has one atom shifted up, and its neighbors shifted down, whereas the β phase the shifts are reversed. Some consequences of this buckling pattern are: i) the increase of spin-orbit coupling, thus enhancing the Quantum Spin Hall Effect; ii) potential to tune several properties with the application of an external electric field. Therefore, the understanding of the effects caused by this buckling is crucial to fully explore the potential of this material. In this work we performed simulations based on Density Functional Theory to investigate the co-existence of the α and β phases in the same sample. We show that: i) This phase inversion is stable in the zigzag and armchair directions, and can make curves, allowing the formation of islands; ii) The formation energy per unit length is approximately 0.02 eV/Ang; iii) The modifications caused in the Density of States (DOS) are small, and appear 0.5 eV below the Fermi energy. Finely, we show how these linear defect will appear in Scanning Tunneling Microscopy (STM) experiments.

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