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Bilayer Silicene: a first principles investigation[1] RENATO BORGES PONTES, Federal University of Goiás, JOSÉ EDUARDO PADILHA, ALDABERTO FAZZIO, ANTÔNIO J.R. DA SILVA, University of São Paulo — By performing ab-initio total energy calculations we study the structural and electronic properties of a silicene bilayer. We show that the lowest energy configuration, contrary to the Bernal stacking of graphene, is when two silicene sheets are placed exactly one on top of the other. In this configuration, there is an energy gain if the system loses its π cloud to create extra (σ-like) chemical bonds between the two layers. To minimize the total energy and the forces that arise due to these new connections made between the layers, the system increases the lattice constant, becoming planar and, consequently, loosing its buckled structure. Moreover, the bilayer of silicene on this planar configuration is a metal and it is insensitive to the presence of an applied external electrical field, a behaviour different from the single layer. We also discuss the role played by the unoccupied 3d-orbital of the silicon in the formation of this new structure. Theoretical STM calculations show excellent agreement with experimental images of silicene bilayers.

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