183 Bilayer Graphene Films on Ru (0001). A Theoretical Study

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Two-dimensional materials have attracted considerable scientific and technological interest [1]. From the scientific point of view they bring the opportunity to test diverse theories on a distinct dimensionality [2,3,4], while their corresponding electronic structure properties suggest several technological applications. Among two dimensional materials, the most widely studied until now is a stable monolayer of graphite: graphene. Nowadays, it is well known that the electronic properties of graphene are strongly modified when it rests on another graphene layer or on a transition metal substrate like the Ru (0001) surface. J. Wintterlin and M. L. Boquet reported graphene adsorbed on metal surfaces. Also, previous investigations have shown that this graphitic structure can consist of few graphene layers (FGL). Thus, as the substrate plays an important role in the electronic properties of graphene, the scientific interest for FGL adsorbed on distinct surfaces has experienced a fast increment in the last years. From a theoretical point of view, single graphene layer and FGL are tractable by means of computational methods involving Tight Binding (TB) and/or Density Functional Theory (DFT) approaches. Thus, in the aim of better understand recent experimental results, we performed DFT calculations for bilayer graphene films over the Ru (0001) surface. Two stacking sequences (AB and AA) for this surface have been considered. For each phase, relaxed atomic positions, calculated Scanning Tunnelling Microscopy (STM) images and density of states (DOS) were obtained and they are revisited with detail.

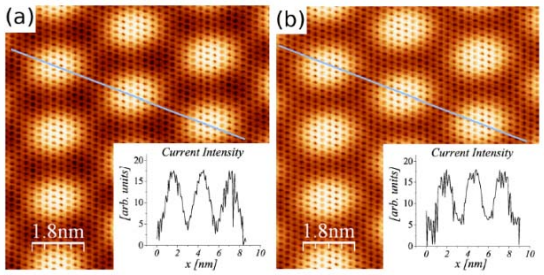

Fig. 1 *Calculated STM images for bilayer graphene over Ru(0001) surface. Stacking AB and AA are presented in (a) and (b) respectively. Bright (dark) regions correspond to high (low) tunnelling current intensity. Insets in each case show line profiles performed along the highlighted segments.*

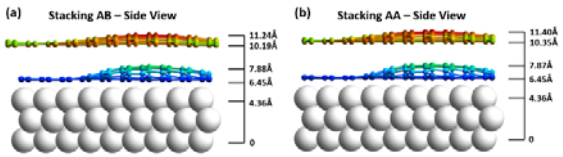

Fig. 2 *Relaxed atomic positions of bilayer graphene over the Ru (0001) surface. Stacking sequences AB and AA are presented respectively.*

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References

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