First-Principles Calculations of Graphene on Ti/Au Surface

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Interaction between graphene (Gr) and metal surface is a fundamental issue for developing Gr based electronic devices. In this paper, we investigated Gr adsorption on Ti/Au surface which is widely used in many transport measurements as a electrode by using the first-principles calculations.
We employed the first principles calulations within PAW-LDA implemented on VASP code. We put Gr on single side of Au, Ti/Au and Ti surfaces consisting 7 atoms layer and introduced 14 Å thich vacuum region. The LDA optimized lattice constants show that Gr 2×2 supercell matches with Au(111) and Ti(0001) $\sqrt{3} \times \sqrt{3}$ surface in comensuration with msmatch 1.7% and -0.7 %.
We found that Gr is weakly adsorbed onto Au surface while it is strongly adsorbed onto Ti and Ti/Au surface. The largest binding energy is realized when Au surface is covered by single monolayer Ti. With monoatomically increase in Ti layers, the physical quantities, such as binding energy and work-function, show strong saturation to those of Ti surface. We also calculate the system with dilute, i.e., less than one-ML, intercalation of Ti between Gr and Au surface and found that charge doping to Gr is strongly suppressed when the conposition of the interface layer is $Ti_{0.33}Au_{0.67}$. Then the potential barrier at Gr and Gr/Ti/Au interface induced by charge doping from metal electrodes is also suppressd and the contact resistance should be small.