

Electron transport characteristics of graphene-metal interfaces

V. Nam Do¹, H. Anh Le¹, and P. Dollfus²

¹Advanced Institute for Science and Technology, Hanoi Univ. of Science and Technology, Vietnam

²Institute of Fundametal Electronics, CNRS, Univ. of Paris-Sud, Orsay, France

e-mail: vannam.do@gmail.com

ABSTRACT

Due to extraordinary properties graphene is expected to become a material of choice for future applications in electronics. However, it has been shown that the interface with metal leads, the indispensable part of any graphene-based device, plays a crucial role in the transport of charges in the whole nanostructure [1-7]. Understanding the phenomena induced by these interfaces may have therefore many technological implications. To tackle this problem from the theoretical point of view, it is mandatory to clarify two issues: (i) the electronic structure of graphene-metal (G-M) complexes at their interfaces, and (ii) the transfer of charges between metal leads and graphene.

To investigate the issue (i), we have used a first-principles approach for five typical G-M complexes, namely G-Cu, G-Au, G-Pt, G-Pd and G-Ti, i.e., for both noble and transition metals. We have used the VASP4.6 package which is based on the projector augmented-wave pseudo-potentials within the general gradient approximation. The resulting electronic structures are shown in Fig. 1. The results show the different effects of metals on the electronic structure of graphene. Metals as Cu and Au just cause slight changes in the electronic structure of graphene and preserve the Dirac cones at the K points. In contrast, in the case of d-bands metal as Pt, Pd and Ti, the graphene electronic structure shares many features with the metal and around the Fermi level we no longer see the typical form of the π -bands of graphene. These results are consistent with the available data obtained by different research groups [8-10].

Regarding the transport issue (ii), the ab initio approach may still be used to explore the transfer characteristics of the G-M interfaces by calculating physical quantities as the conductivity and/or the contact resistivity. However, we have considered a simplified description of sp-bands and d-bands

fitted on first principles-ones, which allows us to study separately the contribution of these bands to the charge transfer through the G-M interface at low computational cost. Our approach, though simple, gives a clear picture of the charge transfer.

We have estimated the intrinsic values of the G-M contact resistivity by exploring the transport in M-G-M structures. Fig. 2 shows the three typical forms of the I-V curves for the five structures. We observe either a negative differential conductance (NDC) for Cu and Au, a positive differential conductance (PDC) for Pt and Pd, or a linear behavior for Ti. Combining these results with the analysis of the band structures leads us to conclude that in the former case (Cu, Au), the Fermi level is far from the d-band edge, the transport is governed by s electrons, which induces an NDC behavior. In contrast, for the G-Ti complex, the Fermi level stays in the middle of the dense d-band and the linear I-V form is understood as that of the regime of wideband limit. Finally, the PDC behavior of the Pt-G-Pt and Pd-G-Pd complexes is attributed to the fact that both the s- and d-electrons contribute to the current but not simultaneously.

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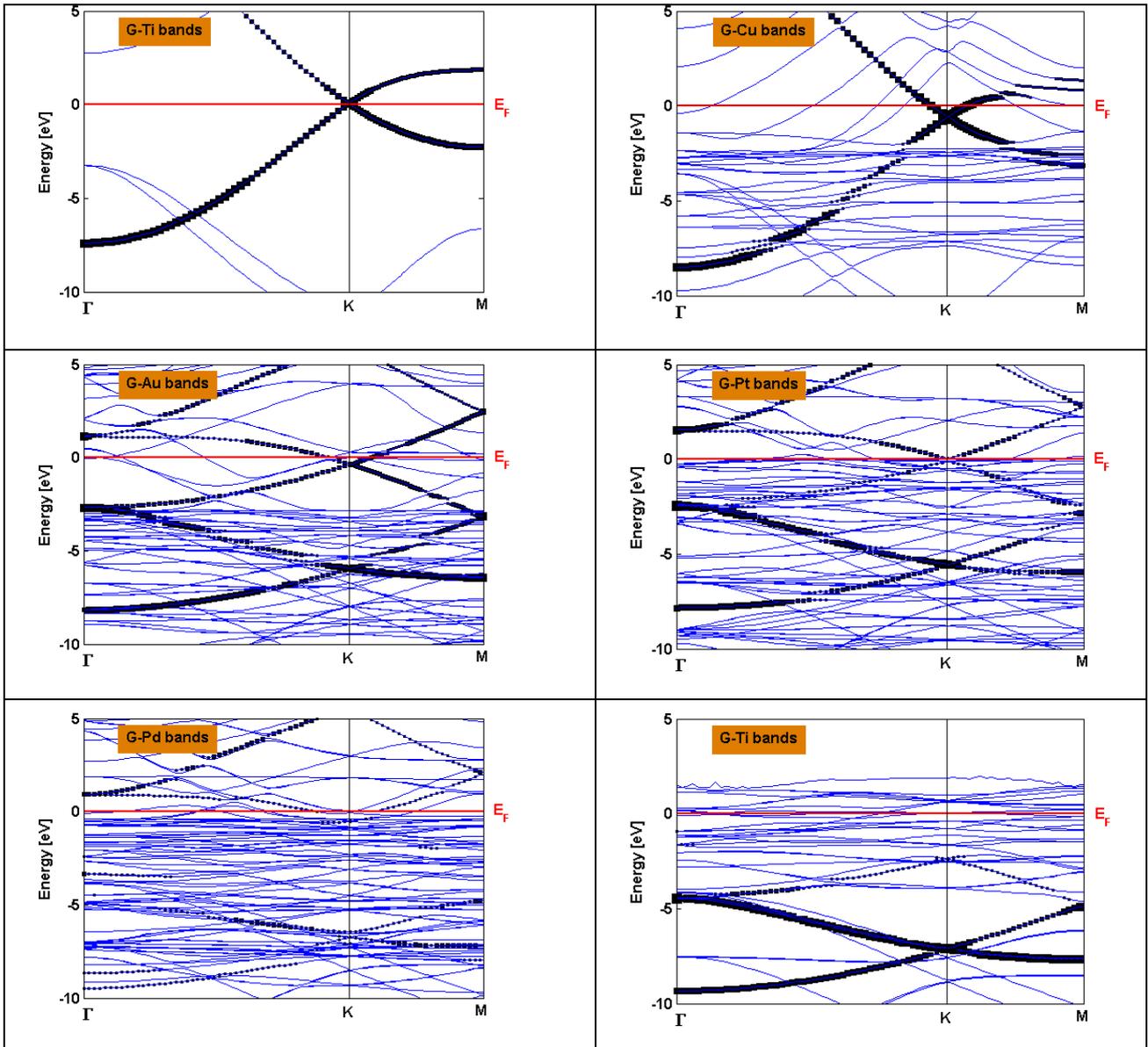


Fig.1. Electronic structure of graphene and of five G-M complexes, i.e. G-Cu, G-Au, G-Pt, G-Pd and G-Ti. The square black symbols guide the eyes to the typical π -bands of graphene formed by the hybridization of carbon p_z -orbitals.

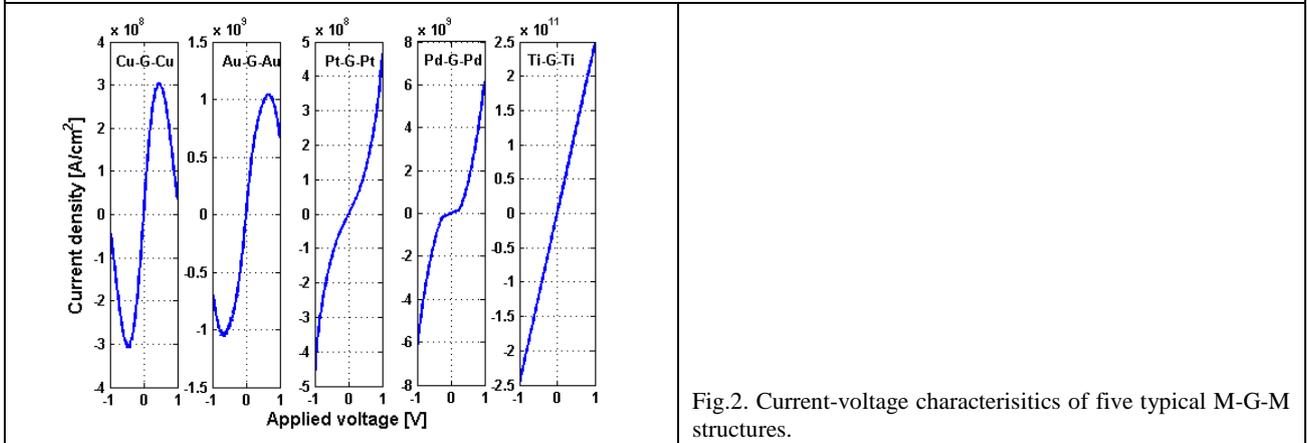


Fig.2. Current-voltage characteristics of five typical M-G-M structures.