CONSIGLIO NAZIONALE DELLE RICERCHE
SHORT-TERM MOBILITY PROGRAMME (YEAR 2008)

Proponent: Prof. Michiel Bertsch
Istituto per le Applicazioni del Calcolo "Mauro Picone" (Bari, Italy)
Recipient: Dr. Valerio Olevano
Institut Néel--CNRS (Grenoble, France)

FINAL REPORT

During the short visit, the recipient has contributed to achieve a relevant result on the investigation of the recently discovered Graphene, an important Condensed Matter system, presenting unusual electronic properties that can be interestingly exploited in Nanoelectronics applications. The work presented by the paper, accepted for publication on Physical Review Letters on October 2008, is of the highest quality and significance for the area of Condensed Matter Physics, both pure and applied, and it is also of broad interest to the general physics community, for all the following reasons.

-The paper deals in particular with the electronic structure of Graphene, that is exactly the feature making Graphene such unusual and interesting: the linear Dirac massless band dispersion; small deviations from the linear dispersion in the form of kinks; finally, the question of the presence or absence of a bandgap at the Dirac point. Two competing experimental groups debate on these issues (A. Bostwick et al. in Nature Physics 3, 36, 2007 and S. Y. Zhou et al. in Nature Materials 6, 770, 2007).

-The work, purely theoretical, is yet linked to the experiment, in particular, to two Angle Resolved Photo-Emission Spectroscopy (ARPES) experiments conducted on the same Berkeley synchrotron facility published by Nature Physics. There authors rise fundamental questions on the kinks and on the bandgap, but their conclusions lead to two completely different scenarios. The paper provides the reader with an *ab initio*, first principle theoretical independent picture, allowing to shed light on the two controversial experimental interpretations.

-The work is a rigorous *ab initio*, first principle theoretical calculation using a state-of-the-art approach, the GW Approximation for the Self-Energy, to take into account electron-electron many body effects, beyond a very simple Tight-Binding or Density-Functional Theory approach. In this purely *ab initio* calculation there is no room for tuning parameters on the experiment: it simulates the full complexity of real Graphene by taking into account its full complicated atomic and electronic structure, that is the effect of all the electrons. In that respect it is predictive.

-The work presents for the first time a theoretical *ab initio* non-adjustable calculation of the Fermi velocity in Graphene. The value calculated is in very good agreement with Magneto-transport experimental findings published by Y. Zhang et al. on Nature 438, 201 (2005). Moreover it finds small kinks (deviations from the linear band dispersion) in stringent agreement with those observed in the experiments. The paper provides a complete theoretical analysis of the nature of such kinks, as due to Many-Body quasi-particle effects, and it supports one of the two experimental interpretations. On the other hand, no bandgap appears at the Dirac point, in striking contrast with the other experimental scenario.

Of course further investigation is needed on Graphene but the ground-breaking message of such a (not ultimate) work is clear: any reliable picture is possible only by having at disposal a robust theoretical approach to the reconstruction of realistic systems. The present collaboration walks along with this creed: the Science to be the ground for both production processes and answers to individual/collective needs. In that respect this research activity meets the stringent criteria of the relevant 7th Framework Programme guidelines issued by the European Union.

In conclusion, the Short-Term Mobility Programme (year 2008) by CNR has supported a fruitful collaboration between two Institutions (CNR--CNRS) sharing the same mission; in that respect, Physical Review Letters is among the highest impact factor (IF) international peer-reviewed journals (IF==7.072 according to the 2006 ISI report). Such a collaboration has been already employed on 2007 and it will continue on 2009.

Both parts wish to keep it in the future in the framework of financed programmes dedicated to this purpose.

Grenoble (France), October 30th 2008

Sincerely Yours

Dr. Valerio Olevano (recipient)