First-Principles simulations of the structure and electronic properties of models of the $\sqrt{13} \times \sqrt{13}$ *R*14° phase of C_{60} on Ge(111)

Eduardo Machado,[1] Pablo Ordejón,[1] Xavier Torrelles,[1] Tien-Lin Lee,[2] Jörg Zegenhagen[2] and Oier Bikondoa[3]

[1]*Institut de Ciència de Materials de Barcelona, CSIC, Campus U.A.B., Bellaterra, 08193 Barcelona (Spain)*
Email: machado@icmab.es, ordejon@icmab.es, xavier@icmab.es
[2]*European Synchrotron Radiation Facility, Polygone Scientifique Louis Néel - 6, rue Jules Horowitz - 38000 Grenoble (France)*
[3]*Department of Chemistry, The University of Manchester, Brunswick Street, Manchester M13 9PL (United Kingdom)*

The structure and properties of C_{60} deposited on surfaces has gathered a great deal of attention during the last years. In the case of Ge(111) surfaces, previous experiments [1-5] have found the existence of three different phases of the deposited C_{60} films. Annealing at high temperatures (500–700°C), yields to a $\sqrt{13} \times \sqrt{13}$ *R*14° phase, in which the distance between C_{60} molecules is ~14.4 Å. This phase has been carefully analysed and characterised [6] using grazing incidence X-ray diffraction, STM and photoemission experiments. The analysis of the X-ray diffraction patterns has allowed proposing models of the atomic structure of the surface.

In this work, we perform first-principles simulation to analyse the models proposed from the X-ray diffraction measurements. Density Functional Theory calculations are used to study the stability of the proposed models, and to give insight into which of them is more stable and therefore more likely to be the best model of the surface. Using the optimised structures, we analyse the electronic properties of the system, and simulate the photoemission spectra and the STM images. We will present a detailed analysis of:

1. The structural models, their stability and relative energies
2. The electronic structure of the different models and the correlation between the features in the electronic spectrum and the structural features (C-Ge bonds, adatoms, etc).
3. The simulated photoemission spectra of each of the models and the comparison with the experimental spectra.
4. The simulated STM images and STS spectra for each of the structural models and their variation with bias voltage. Comparison with the experimental images will also be given.

REFERENCES

[1] H. Xu, D. M. Chen and W. N. Creager, Phys. Rev. B **50**, 8454 (1994)
[2] K. R. Wirth and J. Zegenhagen, Surf. Sci. **351**, 13 (1996)
[3] T. Kidd, R. D. Aburano, H. Hong, T. Gog and T.-C. Chiang, Surf. Sci. **397**, 185 (1998)
[4] A. Goldoni, C. Cepec, M. De Seta, J. Avila, M. C. Asensio and M. Sancrotti, Phys. Rev. B **61**, 15 (2000)
[5] G. Bertoni, C. Cepek and M. Sancrotti, Surf. Sci. **212**, 52 (2003)
[6] X. Torrelles et al, unpublished.

FIGURES

Figure 1. Simulated STM image of a model of the $\sqrt{13} \times \sqrt{13}\ R14^{o}$ phase of C_{60} on Ge(111). The large spherical features are C_{60} molecules, and the small dots in between are Ge adatoms. The simulation was done using the Tersoff-Hamann approximation, with a tip-surface voltage of -2 eV, sampling the occupied states of the surface.