Modelling of the adsorption of C_{60} on the Au(110) surface[1]

Richard J. Baxter,[a,b] Petra Rudolf,[c] Gilberto Teobaldi,[a] Francesco Zerbetto[a]

[a] Dipartimento di Chimica "G. Ciamician", Università di Bologna, Via F. Selmi 2, 40126 Bologna (Italy), Fax: +39 051 2099456, Phone: +39 051 2099473, E-mail: gilberto.teobaldi2@studio.unibo.it; [b] Department of Materials, University of Oxford Parks Road, Oxford OX1 3PH (UK); [c] Materials Science Centre, University of Groningen, Nijenborgh 4, 9747 AG Groningen (The Netherlands).

Abstract

A simple approach based on (i) the glue model for gold,[2] (ii) an empirical force field[3] for C_{60} and (iii) the charge equilibration[4] plus the Born-Mayer potential for their interaction shows that the two experimentally detected structures for C_{60} on Au(110)[5, 6] are competitive from 100 K. The model further shows the different nature of the Au-Au and Au-C_{60} interactions inside the two unit cells, which makes one structure prevail over the other as a function of the experimental conditions. More specifically, the calyx-like structure of ref. [6] is favoured by metal-organic interactions, while the regular structure of ref. [5] is characterized by a remarkable stability of the Au surface.

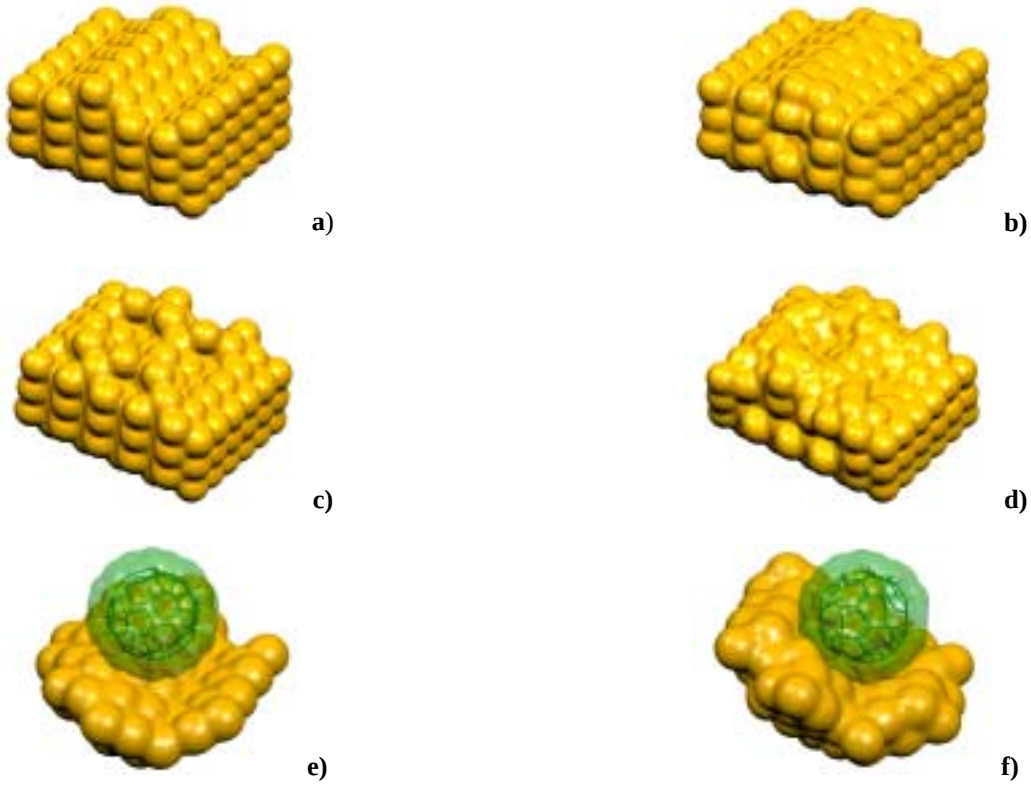

Figure 1: a) the idealized gold overlayer of the structure of ref. [5], b) the optimized gold overlayer of the structure of ref. [5]; c) the idealized gold overlayer of the structure of ref. [6], d) the optimized gold overlayer of the structure of ref. [6]; e) C_{60} on Au(110) following ref. [5] at 300 K, the tips of the arrows indicate the location of the atoms in the ideal icosahedral configuration (the size of the arrows is multiplied by a factor of 10 to assist the eye); f) C_{60} on Au(110) following ref. [6] at 300 K, the tips of the arrows indicate the location of the atoms in the ideal icosahedral configuration (the size of the arrows is multiplied by a factor of 10 to assist the eye).

References

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