Theoretical study of the superatom molecular orbitals of C60-C70

Benoit Mignolet[1], J. Olof Johansson[2], Eleanor E. B. Campbell[2] and Françoise Remacle[1]

[1]Département de Chimie, B6c, Université de Liège, B4000 Liège, Belgium

[2] EaStCHEM, School of Chemistry, University of Edinburgh, West Mains Road, EH9 3JJ, Scotland

bmignolet@ulg.ac.be

fremacle@ulg.ac.be

Recent scanning tunneling microscopy study of C60 on metal surface [1] shows the presence of superatom molecular orbitals (SAMOs). The SAMOs are diffuse hydrogen like orbitals bound to the core of the C60 cage. Photoelectron angular distributions (PADs) of gas-phase C60 and C70 have been obtained by Rydberg fingerprint spectroscopy and angular resolved photoelectron spectroscopy [2]. A rich structure of peaks at low kinetic energies is observed and the angular distributions of these peaks are compared with theoretical PADs. From the Dyson orbital of a large band of 500 excited states of C60 and C70 computed in time dependent density functional theory, we computed the energy dependence of the PADs of the randomly oriented excited states with respect to the electron kinetic energy (fig. 1). The excited states composed of the SAMOs have high ionization probabilities and specific angular distributions that are in good agreement with the experimental results.

References:

[1] M. Feng, J. Zhao, and H. Petek, Science, 320 (2008) 359.

[2] J. O. Johansson, G. G. Henderson, F. Remacle, and E. E. B. Campbell, Physical Review Letters, 108 (2012) 173401.

Figures:

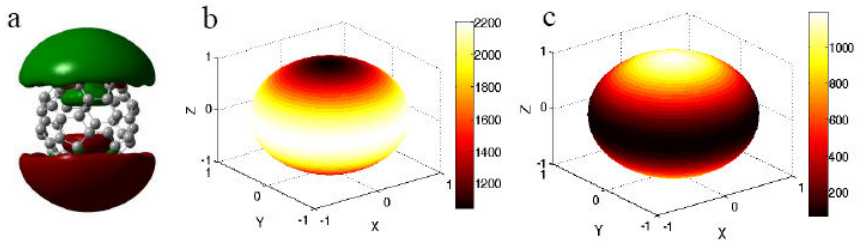

Figure 1: (a) Dyson orbital of the excited state 287 of C60. (b)-(c) Computed photoelectron angular distribution of the randomly oriented band of excited states close in energy of the exited state 287 for a kinetic energy of 0.1eV (b) and 1.3eV(c).