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Molecular Calculations of the Photoionization of Endohedral Atoms: Ar@C_{60} A. PONZI, M. STENER, P. DECLEVA, Universita' di Treste, S.T. MANSON, Georgia State University — Endohedral fullerenes represent a particularly clean case of quantum confinement where the electronic properties of the guest atom or molecule are strongly modified by the encapsulating host.. Many theoretical studies, e.g [1-5], have been performed both on free C_{60} and endohedral systems, and the predicted confinement resonances have been confirmed by recent experiment [6]. Most calculations have employed jellium models for the C_{60} moiety, allowing the treatment of electron response effects and interchannel coupling [4,5], while the few molecular calculations have been limited to a static description, either at the DFT [1,2] or static-exchange level [5], giving, however, some conflicting evidence with interpretations based on jellium treatments. The development of large scale TDDFT codes [7] allows full treatment of nonspherical and response effects, and this methods is applied to Ar@C_{60}, to compare with results and assess the modifications brought about by the full inclusion of the ionic cores. It is found that molecular effects increase hybridization of the atomic orbitals with the cage and reduces the role of response effects, due to the stronger localization of the electron cloud. [1] P. Decleva *et al*, *J. Phys. B* **32**, 4523 (1999); [2] P. Colavita *et al*, *Phys. Chem. Chem. Phys.* **3**, 4481 (2001); [3] M. E. Madjet *et al*, *Phys. Rev. Lett.* **99**, 243003 (2007); [4] T. W. Gorczyca *et al*, Phys. Rev. A **86**, 033204 (2012); [5] J. Jose and R. R. Lucchese, *J. Phys. B* **46**, 215103 (2013); [6] R. A Phaneuf *et al*, Phys. Rev A, **88**, 053402 (2013); [7] M. Stener *et al, J. Chem. Phys.* **122**, 234301 (2005).

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