Abstract Submitted
for the DAMOP18 Meeting of
The American Physical Society

Photoionization of C_{60}: Effects of correlation on cross sections and angular distributions of valence subshells A. PONZI, P. DECLEVA, Universit di Trieste, S. T. MANSON, Georgia State University — Calculations of the photoionization of all of the 32 valence subshells, from the outermost $6h_u$ to the innermost $2a_g$, of the free C_{60} molecule have been performed using a time-dependent density function theory (TDDFT) methodology within the framework of a fully molecular model [1]. Cross sections and photoelectron angular distribution β parameters have been obtained and the results have been broadened to simulate vibrational structure. In addition, the calculations are performed at the ordinary density functional theory (DFT) level, basically central-field calculations, in an effort to understand the role of correlation in the photoemission process. The spectra are fraught with narrow autoionizing and shape resonances which make then quite difficult to analyze, along with the much broader confinement resonances [2]. The narrow shape resonances show up quite clearly in the photoionization at energies above the lowest $2a_g$ threshold and in the $2a_g$ cross section itself where autoionization is not possible. [1] A. Ponzi, P. Decleva and S. T. Manson, Phys. Rev. A 92, 023405 (2015); [2] J.-P. Connerade, V. K. Dolmatov and S. T. Manson, J. Phys B **33**, 2279 (2000).

Steven Manson
Georgia State University

Date submitted: 06 Feb 2018 Electronic form version 1.4