Abstract Submitted
for the GEC14 Meeting of
The American Physical Society

Single photoionization of many electron atoms and molecules: a Sturmian approach. CARLOS M. GRANADOS CASTRO, LORENZO UGO ANCARANI, Universite de Lorraine, Metz, France, DARIO M. MITNIK, IAFE, Buenos Aires, Argentina, GUSTAVO GASANEO, Universidad Nacional del Sur, Bahia Blanca, Argentina — The Sturmian approach, using Generalized Sturmian Functions (GSF), has been applied successfully for the study of several atomic ionization processes [1]. The extension of the method to molecular systems is under development, and is the subject of the present contribution. As a first step, in order to test our methodology, we started with some atomic systems and calculated the photoionization cross section using the one-active electron approximation together with model potentials. We solved the time-independent, first-order perturbative, Schrödinger equation; the scattering wave function is expanded in GSF. Having validated our approach and computer codes, we then studied the photoionization of molecules, such as CH_4, using a similar method. After considering initially an angular-averaged model potential, we then used a non-central one leading to a set of angular-coupled of equations. The scattering wave function is again expanded in a GSF basis set, but this time with many different angular momenta. In order to take into account the random orientation of the molecule, an angular average over all the possible spatial orientation of the molecule is finally performed. The calculated cross sections are compared with theoretical and experimental data (see [2] and references therein).

[1] G. Gasaneo et al, Adv. Quantum Chem. 67, 153 (2013).
[2] C. M. Granados-Castro et al, Few-Body Systems, in press (2014).

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Date submitted: 16 Jun 2014 Electronic form version 1.4