Abstract Submitted
for the GEC15 Meeting of
The American Physical Society

Electron impact ionization of CH_4, H_2O and NH_3 with a Sturmian approach[1] LORENZO UGO ANCARANI, CARLOS MARIO GRANADOS-CASTRO, Université de Lorraine, France, DARIO M. MITNIK, IAFE, Buenos Aires, Argentina, GUSTAVO GASANEO, Universidad Nacional del Sur, Argentina
— The study of ionization of molecular systems is more complex and challenging than in the atomic case because the Hamiltonian is generally multicenter and highly non-central. Additionally, in most experiments the molecular spatial orientation is not resolved, so that the random orientation of the molecule must be taken into account through an adequate angular average. In this contribution, we illustrate our implementation of a Sturmian approach, based on Generalized Sturmian Functions [1], for the study of single electron impact ionization of small molecules. Molecular model potentials are proposed to describe the interaction between the ejected electron with the parental ion. A similar approach was used before to study photoionization of molecules [2]. The calculated triple differential cross sections for ionization from valence orbitals of CH_4, NH_3 and H_2O will be reported, and compared with different available theoretical and experimental data.

[1] G. Gasaneo et al, Adv. Quantum Chem. 57, 153 (2013).
[2] C. M. Granados-Castro, Adv. Quantum Chem. (2015), accepted for publication.

[1]We acknowledge the CNRS (PICS project N. 06304) and CONICET (project N. Dl 158114) for funding our French-Argentinian collaboration.

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Date submitted: 17 Jun 2015 Electronic form version 1.4