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Sturmian approach to the study of photoionization of atoms and molecules CARLOS MARIO GRANADOS CASTRO, LORENZO UGO ANCARANI, Universite de Lorraine, France, GUSTAVO GASANEO, Universidad Nacional del Sur, Argentina, DARIO M. MITNIK, IAFE, Buenos Aires, Argentina — In this presentation we study the photoionization of atoms and molecules using ultrashort laser pulses, solving the time-independent Schrödinger equation (TISE) in a first order perturbation theory. The interaction laser-matter is described with the dipolar operator in the velocity gauge. Generalized Sturmian functions [1] are used to solve the driven equation for a scattering wave function which includes all the information about the ionization problem. For the atomic case, we study the photoionization of He atom using the Hermann-Skillman potential together with the one-active electron approximation. For molecular systems (CH_4 in this work), we use first a spherically symmetric potential $U_i(r)$ [2], and then a more realistic potential that includes all the nuclei and other electrons interaction, as in [2]. For each molecular orbital we use Moccia's wave functions [3], solve the TISE with an initial molecular orbital i of the ground state and extract the corresponding photoionization cross sections. For both atomic and molecular systems we compare our results with previous calculations and available experimental data.

[1] D. M. Mitnik et al, Comp. Phys. Comm. 182, 1145 (2011); Gasaneo et al, submitted to Adv. Quantum Chem (2013)
[2] L Fernandez-Menchero and S Otranto, Phys. Rev. A 82 022712 (2010)
[3] R Moccia, J. Chem. Phys. 40 2164. (1964)

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