

Abstract Submitted
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The role of nuclear dynamics in molecular ionization processes produced by synchrotron radiation and ultrashort pulses FERNANDO MARTIN, Departamento de Quimica. C-9. Universidad Autonoma de Madrid. 28049-Madrid. Spain. — The important role of nuclear dynamics in molecular ionization processes produced by synchrotron radiation and ultrashort pulses will be demonstrated using accurate ab initio theoretical calculations that account for all electronic and vibrational degrees of freedom. Results for electron angular distributions from fixed-in-space H₂ molecules will be presented. For photon energies of a few hundreds of eV, it is shown that, for molecules oriented parallel to the polarization direction, the angular patterns reveal a complex nodal structure, while for molecules oriented perpendicularly, typical Young's double-slit interferences are observed. These patterns change dramatically as the molecule vibrates. For photon energies of ~ 30 eV, it is shown that the emission of a photoelectron with subsequent dissociation of the remaining H₂⁺ fragment shows no symmetry with respect to the ionic H⁺ and neutral H atomic fragments. This lack of symmetry results from the entanglement between symmetric and antisymmetric H₂⁺ states caused by autoionization. The dependence on pulse parameters of multiphoton ionization of H₂ by ultrashort pulses will also be analyzed. Refs: A. Palacios et al, Phys. Rev. Lett. **96**, 173201 (2006); J. Fernández et al, Phys. Rev. Lett. **98**, 043005 (2007); F. Martín et al, Science **315**, 630 (2007).

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