

Abstract Submitted
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Light-induced and Natural Nonadiabatic Phenomena in Diatomics¹ AGNES VIBOK, ANDRAS CSEHI, University of Debrecen, LORENZ CEDERBAUM, University of Heidelberg, GABOR HALASZ, University of Debrecen, UNIVERSITY OF DEBRECEN COLLABORATION, UNIVERSITY OF HEIDELBERG COLLABORATION — Nonadiabatic effects play a very important role in controlling chemical dynamical processes. They are strongly related to avoided crossings (AC) or conical intersections (CIs) which can either be present naturally or induced by classical or quantized laser light ("light-induced avoided crossings" (LIACs) and "light-induced conical intersections" (LICIs)). In the latter situation the radiation field mixes the nuclear and electronic degrees of freedom in an optical cavity. Here we show to what extent the classical or cavity's quantized field description of the electric field are equivalent. Solving the time-dependent nuclear Schrödinger equation we can simulate either LIAC or LICI situations in the NaI molecule, which is a strongly coupled diatomic in field free case. Obtained results undoubtedly demonstrate a significant difference between the impact of the LIAC and that of the LICI on the dynamics of the molecule, as well as the collective effect of light-induced and natural nonadiabatic phenomena.

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