Accepted Manuscript

Collective effect of light-induced and natural nonadiabatic phenomena in the dissociation dynamics of the NaI molecule

András Csehi, Gábor J. Halász, Ágnes Vibók

PII:	S0301-0104(17)30908-4
DOI:	https://doi.org/10.1016/j.chemphys.2017.12.017
Reference:	CHEMPH 9898
To appear in:	Chemical Physics
Received Date:	28 October 2017
Accepted Date:	29 December 2017



Please cite this article as: A. Csehi, G.J. Halász, A. Vibók, Collective effect of light-induced and natural nonadiabatic phenomena in the dissociation dynamics of the NaI molecule, *Chemical Physics* (2017), doi: https://doi.org/10.1016/j.chemphys.2017.12.017

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Collective effect of light-induced and natural nonadiabatic phenomena in the dissociation dynamics of the NaI molecule

András Csehi(1),(2), Gábor J. Halász(3) and Ágnes Vibók(1),(2)*,[†]

†(1)Department of Theoretical Physics, University of Debrecen, H-4002 Debrecen, PO Box 400, Hungary

 ‡(2) ELI-ALPS, ELI-HU Non-Profit Ltd, H-6720 Szeged, Dugonics tér 13, Hungary
¶(3)Department of Information Technology, University of Debrecen, H-4002 Debrecen, PO Box 400, Hungary

E-mail: vibok@phys.unideb.hu

Abstract

Natural and light-induced nonadiabatic effects are ubiquitous in many photochemical and photophysical processes. Here we study the interplay between them when they are present simultaneously in a molecular system. Our showcase example is the NaI molecule. Solving the time-dependent nuclear Schrödinger equation the photodissociation rate and the angular distribution of the molecular photofragments are calculated and discussed at several resonant laser energies and intensities. Obtained results clearly demonstrate that the dissociation rate and the angular distribution of the NaI photofragments can be considered as clear fingerprint of a collective effect of light-induced and natural nonadiabatic phenomena.

Keywords: photodissociation;

nonadiabatic coupling term; external electric field; light-induced nonadiabatic phenomena; Download English Version:

https://daneshyari.com/en/article/7837140

Download Persian Version:

https://daneshyari.com/article/7837140

Daneshyari.com