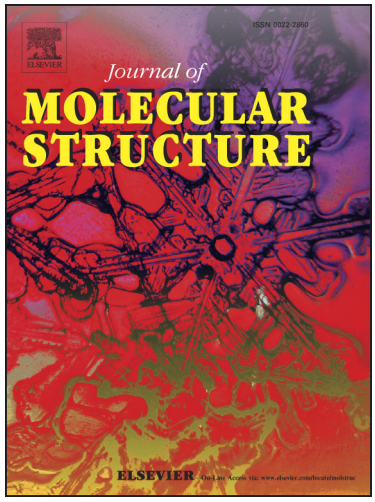

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Optimal control of dissociation of nitrogen molecule with intense ultra-short laser pulse shaping

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Abstract

The quantum optimal control theory in conjunction with time dependent density functional theory is used to optimize the laser pulse shape for dissociation of nitrogen molecule. For several initial peak intensities and frequency ranges, the optimum shapes are produced and compared to determine the most efficient pulse. Ehrenfest molecular dynamics model is also used to test the dissociation process. The corresponding snapshots of density and time dependent electron localization function are presented. It is noticed that when the frequency ranges of laser pulses are doubled, it leads to 60% faster dissociation of N_2 molecule.

Keywords: nitrogen molecule, dissociation, time dependent density functional theory, optimal control theory, pulse shaping.

I. Introduction

Controlling the dynamics of quantum systems and chemical bonds with optimized laser pulses is a main goal in physics and chemistry. Intense femtosecond laser pulses and weak extreme ultraviolet attosecond pulses are developed to facilitate these phenomena in the interesting subjects such as determination of optimal fields capable of dissociation, controlling and monitoring of electron dynamics in real time and also laser and matter interaction field [1-4].

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