ELECTRON-IMPACT INDUCED MOLECULAR DYNAMICS WITHIN THE ATMOLCOL FRAMEWORK

Sanja Tošić[1], Vladimir A. Srećković[1], Veljko Vujčić[2]

[1]University of Belgrade, Institute of Physics Belgrade, , Pregrevica 118, Belgrade, Serbia, seka@ipb.ac.rs, vlada@ipb.ac.rs,
[2]Astronomical Observatory, Volgina 7, 1100 Belgrade, Serbia, veljko@aob.rs

ABSTRACT

Within the ATMOLCOL project, experimental investigations of electron–molecule collisions increasingly require theoretical input capable of clarifying the molecular mechanisms that lead to fragmentation. The work presented here contributes to this effort through the development of a computational model aimed at simulating fragmentation of molecular cations formed from their ground-state electronic configurations. The primary scattering event is not treated explicitly. Instead, attention is directed to the nuclear dynamics that follow electronic perturbation, under internal energy conditions consistent with experimentally accessible regimes. Molecular dynamics simulations are used to examine dissociation pathways, locate transition structures, and estimate the corresponding activation energies. Particular care is devoted to numerical stability and to ensuring that the identified fragmentation channels are not artifacts of trajectory sampling or insufficient exploration of the potential energy surface. At the current stage, the methodology is tested on the N_2^+ molecular cation as a representative diatomic benchmark system. Although structurally simple, this system provides a controlled reference for analyzing bond cleavage and verifying energy conservation during dynamical propagation. It also allows systematic assessment of the model before extension to larger polyatomic molecules, where energy redistribution and competing pathways are expected to become more intricate. This work represents a methodological contribution toward a quantitative description of radiation-induced molecular fragmentation within ATMOLCOL project.

Keywords: electron–molecule collisions, fragmentation pathways, molecular dynamics, short-time processes.

Acknowledgments

This research was supported by the Science Fund of the Republic Serbia, Grant No. 6821, ATMOLCOL.