POST-COLLISION MOLECULAR DYNAMICS OF ELECTRON-IMPACT IONIZED MOLECULAR CATIONS

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ABSTRACT

Within the ATMOLCOL project, experimental studies of electron–molecule collisions increasingly rely on theoretical models that can clarify the molecular mechanisms leading to fragmentation. This work contributes by developing a computational approach to simulate the fragmentation of molecular cations originating from their ground-state electronic configurations. The primary electron–molecule scattering event is not modeled explicitly; instead, the focus is placed on post-collision nuclear dynamics under internal energy conditions relevant to experiments. Molecular dynamics simulations are employed to analyze dissociation pathways, identify transition structures, and estimate activation energies. Particular attention is given to numerical stability and to verifying that the observed fragmentation channels are not artifacts of limited trajectory sampling or insufficient exploration of the potential energy surface. At this stage, the methodology is tested on the N_2^+ molecular cation as a benchmark diatomic system. Despite its simplicity, N_2^+ provides a well-controlled reference for studying bond cleavage, monitoring energy conservation during dynamical propagation, and validating the robustness of the approach. This benchmark assessment is a necessary step before extending the model to larger polyatomic systems, where energy redistribution and competing fragmentation pathways become more complex. Overall, the study represents a methodological contribution toward a quantitative description of radiation-induced molecular fragmentation within the ATMOLCOL framework.

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

INTRODUCTION

Low-energy electron–molecule collisions play a central role in a wide range of physical and chemical environments, including cold plasmas, planetary and interstellar media, atmospheric

processes, and radiation-driven chemistry [1-5]. In many of these systems, electron impact leads not only to electronic excitation or ionization, but also to molecular fragmentation, dissociation, and energy redistribution among nuclear degrees of freedom [6, 7]. A reliable theoretical interpretation of such processes therefore requires a consistent description of the post-collision nuclear dynamics following the initial electron–molecule interaction [8, 9].

Within the ATMOLCOL framework, electron–molecule collisions are typically treated as a two-step process. In the first step, the electronic interaction between the incident electron and the target molecule leads to excitation, attachment, or ionization, often described using quantum scattering methods. In the second step, the system evolves on one or more potential energy surfaces, during which nuclear motion governs bond stretching, vibrational excitation, and eventual fragmentation. While the electronic dynamics are frequently well captured by state-of-the-art scattering calculations, the subsequent nuclear motion is often treated using simplified or implicit models, despite its crucial role in determining observable fragment distributions.

Fragmentation observables, such as kinetic energy release, angular distributions, and branching ratios between different dissociation channels, are inherently sensitive to the time-dependent nuclear dynamics after the collision. In particular, energy deposited during the electron impact is redistributed among vibrational modes on ultrafast time scales [10], and even small inaccuracies in the description of this redistribution can lead to significant deviations in predicted fragment yields [11]. This makes post-collision nuclear dynamics a key ingredient for connecting microscopic collision mechanisms to experimentally accessible observables.

Classical and semiclassical molecular dynamics approaches provide a natural and computationally efficient framework for modeling nuclear motion following electron impact, especially when the focus lies on qualitative trends, methodological validation, or large-scale simulations involving many trajectories. In this context, it is essential to establish robust and numerically stable integration schemes that accurately conserve energy and preserve the phase-space structure of the system over long propagation times. Such validation is particularly important before extending the approach to more complex, multidimensional molecular systems relevant for ATMOLCOL applications.

In this work, we present a methodological study of post-collision nuclear dynamics. Post-collision nuclear motion is modeled classically on a one-dimensional Morse potential, with the impact of the electron incorporated through the initial internal energy. The equations of motion are integrated using the Velocity Verlet algorithm over 5000 time steps to ensure numerical stability and energy conservation. Simulations are performed using a modular in-house code optimized for efficient trajectory propagation and energy monitoring. Computations are carried out on a high-performance workstation equipped with modern multi-core processors and dedicated graphical processing units (GPUs), enabling scalable extension to multidimensional and ensemble-based simulations.

The present study is intended as a foundational step toward incorporating impact-induced nuclear dynamics into the ATMOLCOL framework, providing a controlled environment for testing integration schemes and analyzing their suitability for modeling fragmentation processes in electron–molecule collisions.

THEORETICAL MODEL

The post-collision nuclear dynamics is described within a classical framework, where the motion of the nuclei evolves on an effective potential energy surface corresponding to the electronically perturbed molecular state. Such approach is commonly adopted when the primary electron-molecule interaction is treated separately and the focus lies on the subsequent redistribution of energy among nuclear degrees of freedom. In this regime, classical and semiclassical trajectory methods have proven to be effective tools for capturing vibrational motion, bond stretching and dissociation dynamics, provided that the underlying potential energy surface accurately represents the relevant anharmonic features of molecular binding [12-14]. For a controlled methodological study, we consider a one-dimensional diatomic model represented by

the Morse potential, which captures essential features of molecular binding and anharmonicity while remaining numerically transparent.

The interaction potential is given by

$$V(x) = D\left[1 - e^{-a(x-x_0)}\right]^2$$

where D is the dissociation energy, a determines the curvature of the potential well, and x, x_0 denotes the equilibrium internuclear separation. Although simplified, the Morse potential provides a realistic description of bond stretching and dissociation and is therefore well suited for benchmarking molecular dynamics schemes intended for fragmentation studies [15]. Recent work has further demonstrated that simple analytical potentials can serve as reliable effective models when validated against ab initio potential energy surfaces, particularly in methodological and benchmarking contexts [16].

The nuclear motion is governed by Newton's equation of motion,

$$m\frac{d^2x}{dt^2} = -\frac{dV(x)}{dt}$$

where m m is the reduced mass of the diatomic system. The force acting on the nuclei is obtained analytically from the derivative of the Morse potential, allowing for stable and efficient numerical propagation. Such classical trajectory approaches have been shown to reproduce key aspects of vibrational energy redistribution and bond dynamics following electronic excitation and ionization, especially when the emphasis lies on qualitative trends and numerical stability rather than fully quantum-resolved distribution [13, 17]

In the present work, the primary electron–molecule collision is not treated explicitly. Instead, its effect is incorporated through the choice of initial conditions and internal energy, consistent with the post-collision regime probed in electron-impact experiments. This separation allows us to focus on validating the nuclear dynamics model and its suitability for describing fragmentation processes within the ATMOLCOL framework.

NUMERICAL METHOD

The time evolution of the nuclear motion is obtained by numerically integrating Newton's equation of motion using the Velocity Verlet algorithm, a standard integration scheme in molecular dynamics simulations. This algorithm is particularly well suited for conservative systems, as it is time reversible and symplectic, ensuring good long-term stability and accurate energy conservation [18]. Early formulations of Verlet-type integration were introduced to preserve Hamiltonian structure of the equations of motion, laying the foundation for modern molecular dynamics integrators [19].

For a given position x_i_and velocity v_i at time t_i, the position at the next time step is updated according to

$$x_{i+1} = x_i + v_i\Delta t + \frac{1}{2}a_i\Delta t^2$$

where $a_i = \frac{F(x_i)}{m}$ is the acceleration derived from the Morse force. The velocity is then updated using

$$v_{i+1} = v_i + \frac{1}{2}(a_i + a_{i+1})\Delta t$$

where a_{i+1} is evaluated at the new position x_{i+1}. These update rules ensure that energy drift remains bounded over long simulations and that phase-space structure is preserved, properties that have been emphasized in recent assessments of classical MD schemes [20].

The simulations are performed in reduced units, where the reduced mass is set to m =1.0 and a fixed time step Δt=0.01 is given in corresponding dimensionless time units. The trajectories are propagated for N=5000 time steps, corresponding to a total simulation time sufficient to assess the stability of bound motion and energy conservation. Initial conditions are chosen such that the system remains within the Morse potential well, allowing for controlled analysis of oscillatory dynamics.

The numerical implementation explicitly stores the time evolution of position, velocity, potential energy, and total mechanical energy. This enables a direct assessment of numerical accuracy through monitoring of energy conservation and phase-space structure, which is essential before extending the approach to impact-induced fragmentation scenarios.

RESULTS

As a first validation step, the numerical scheme is applied to a diatomic benchmark system representing the nuclear motion of the N^{2+} molecular cation. Diatomic systems provide a controlled testing ground for post-collision nuclear dynamics, as they allow direct monitoring of bond stretching, energy redistribution, and phase-space structure without the additional complexity of multidimensional mode coupling present in larger molecules [21]. Classical trajectory studies have similarly employed diatomic benchmarks to assess numerical stability and vibrational energy flow [22], while recent work on N_2^+ dissociative processes highlights the relevance of accurate post-collision to experimentally observable fragmentation [23]. This makes them particularly suitable for methodological studies aimed at validating integration schemes prior to extension to polyatomic targets relevant for ATMOLCOL.

The nuclear motion is propagated on a Morse potential surface, shown in Fig. 1, which models the effective potential energy surface of the electronically perturbed molecular ion. For the chosen initial conditions, the system remains in a bound dynamical regime, executing anharmonic oscillatory motion around the equilibrium position. This regime is representative of post-collision situations in which the energy deposited by electron impact is insufficient to induce immediate dissociation but leads to significant vibrational excitation. The anharmonic shape of the potential allows for a realistic description of bond stretching and provides a suitable benchmark for post-collision nuclear dynamics.

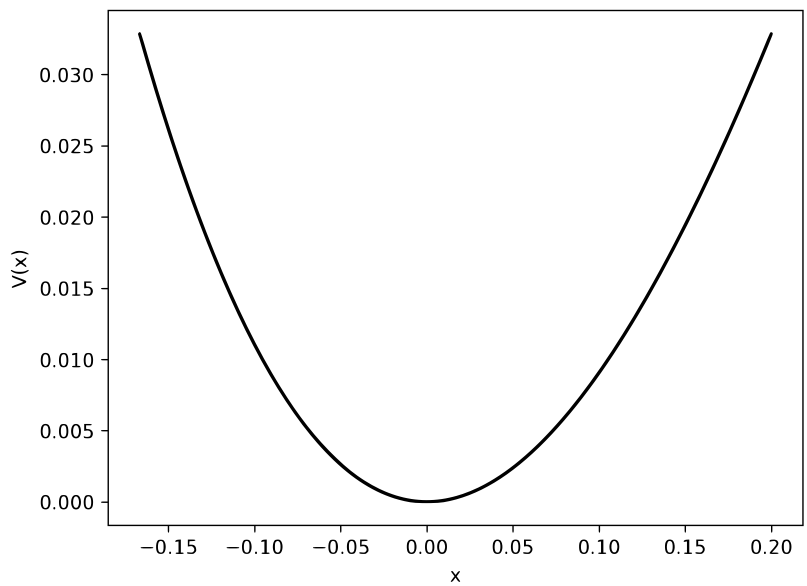


Figure 1. Morse potential V(x) used to model the effective potential energy surface of the diatomic molecular cation.

The time evolution of the total mechanical energy is shown in Fig. 2. The energy remains nearly constant throughout the simulation, with small oscillations around a mean value and no systematic drift. The apparent oscillations are of numerical origin and remain at the 10^{-6} level relative to the mean energy. The absence of systematic drift indicates stable numerical propagation using the Velocity Verlet integration scheme. To quantify the numerical stability, the deviation of the total energy from its mean value is plotted in Fig. 3, demonstrating that fluctuations remain well below the 10^{-4} level over the full propagation time. This confirms that the chosen time step and integration scheme are adequate for describing post-collision nuclear dynamics on the relevant time scales.

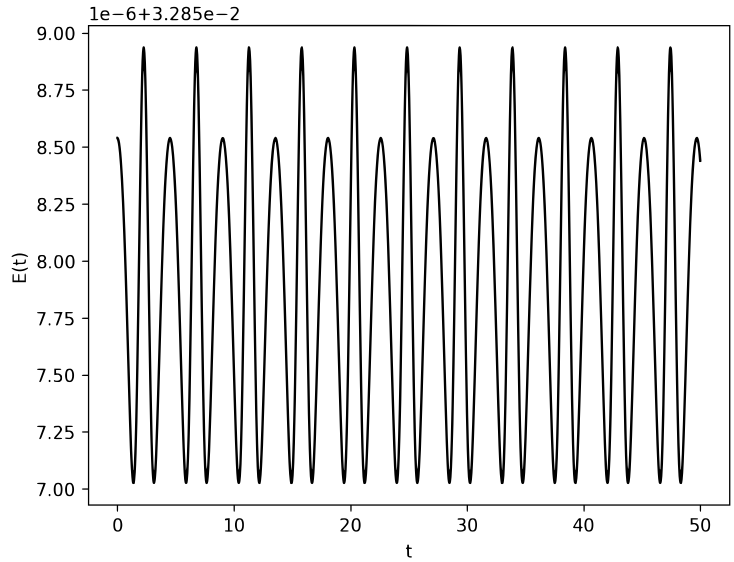


Figure 2. Time evolution of the total mechanical energy E(t) for bound nuclear motion on the Morse potential.

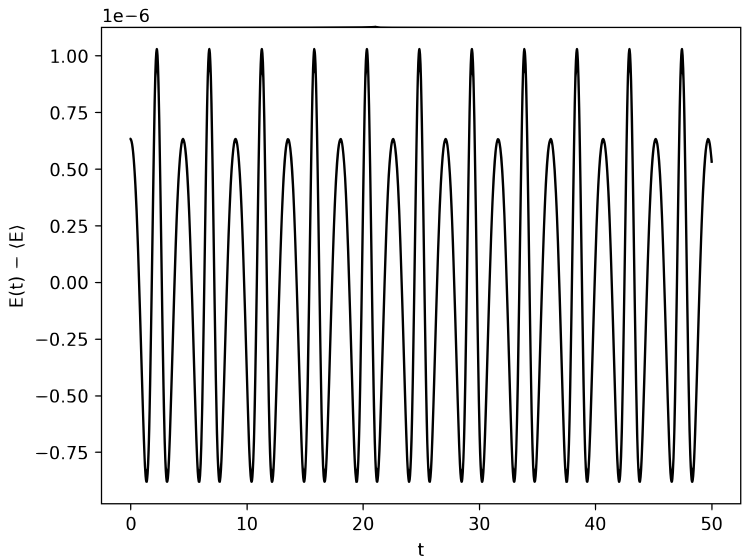


Figure 3. Deviation of the total mechanical energy from its mean value, E(t)−⟨E⟩ over the full simulation time.

Further insight into the dynamical behavior is obtained from the phase-space trajectory (x,v), shown in Fig. 4. The closed, regular orbit indicates stable bound motion and preserves the expected phase-space structure of an anharmonic oscillator. The absence of distortion or secular spreading in phase space further validates the symplectic character of the Velocity Verlet integrator and its suitability for extended molecular dynamics simulations.

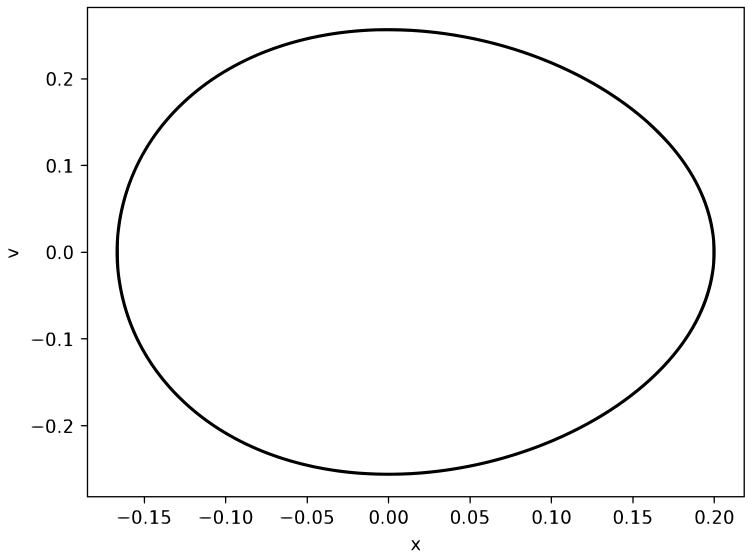


Figure 4. Phase-space trajectory (x,v) corresponding to bound nuclear motion in the Morse potential.

DISCUSSION

The results presented above demonstrate that the adopted molecular dynamics scheme provides a stable and physically consistent description of post-collision nuclear motion on an effective potential energy surface. Although the primary electron–molecule interaction is not treated explicitly, the present approach captures the essential features of the nuclear dynamics that follow electronic excitation or ionization, which are directly relevant for the interpretation of fragmentation phenomena investigated within the ATMOLCOL project.

In electron–molecule collisions, the energy transferred during the impact is rapidly redistributed among nuclear degrees of freedom, governing whether the system remains bound, undergoes vibrational excitation, or proceeds toward dissociation. The bound dynamical regime analyzed here corresponds to post-collision conditions below the effective dissociation threshold, where nuclear motion remains confined but highly sensitive to the amount of deposited internal energy. Accurate modeling of this regime is a prerequisite for understanding the transition to fragmentation at higher excitation energies.

The excellent energy conservation and preserved phase-space structure observed in the present simulations confirm that the Velocity Verlet integrator is well suited for describing such post-collision nuclear dynamics over extended propagation times, in agreement with recent benchmark studies emphasizing numerical stability in molecular dynamics simulations [24]. This is particularly important for impact-induced processes, where small numerical artifacts may accumulate and lead to artificial dissociation or unphysical energy drift, thereby compromising the interpretation of experimental observables.

While the present study is restricted to a one-dimensional diatomic benchmark, it establishes a controlled reference framework for extending the approach to more complex molecular systems.

In polyatomic targets, additional degrees of freedom will introduce energy redistribution among vibrational modes and competing fragmentation pathways. The validated numerical stability demonstrated here provides confidence that such effects can be explored systematically by extending the model to multidimensional potential energy surfaces and ensemble-based simulations.

Within the ATMOLCOL framework, the present methodology offers a practical route for coupling electronic scattering calculations with post-collision nuclear dynamics. By providing a transparent and numerically robust description of nuclear motion following electron impact, the approach represents a foundational step toward quantitative modeling of electron-induced molecular fragmentation.

CONCLUSION

In this work, a classical molecular dynamics framework has been developed and validated for the description of post-collision nuclear dynamics relevant to electron–molecule interactions within the ATMOLCOL project. By focusing on the nuclear motion following electronic excitation or ionization, the present approach addresses a key component required for the interpretation of fragmentation processes induced by electron impact.

Using a diatomic benchmark system modeled by a Morse potential, we have demonstrated that the Velocity Verlet integration scheme provides stable numerical propagation with excellent energy conservation and preservation of phase-space structure. These properties are essential for reliable simulations of post-collision dynamics, where small numerical inaccuracies may otherwise lead to artificial dissociation or unphysical energy redistribution.

Although the present study is restricted to bound nuclear motion in a one-dimensional model, it establishes a controlled methodological reference for future extensions. In particular, the framework can be naturally generalized to higher-dimensional systems and polyatomic molecules, where multiple vibrational degrees of freedom and competing fragmentation pathways play a dominant role. The validated numerical stability achieved here provides confidence that such extensions can be pursued without compromising physical consistency.

Within the ATMOLCOL framework, the present results represent a foundational step toward coupling electronic scattering calculations with post-collision nuclear dynamics. The approach offers a transparent and computationally efficient route for modeling post-collision molecular dynamics following electron impact, and paves the way for future studies addressing dissociative regimes, threshold behavior, and complex molecular targets.

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DECLARATIONS OF INTEREST STATEMENT

The authors affirm that there are no conflicts of interest to declare in relation to the research presented in this paper.

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