Investigation of electron and ion dynamics in small hydrocarbons subjected to laser pulses

Ruben Medina[1], Sergiy Bubin[2], & Kalman Varga[2]

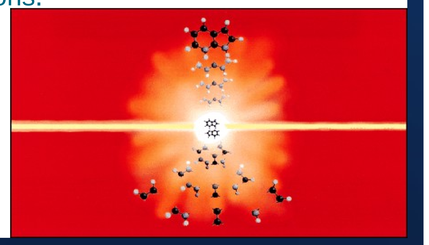
[1] Department of Physics, California State University - Dominguez Hills, Carson, CA 90747

[2] Department of Physics, Vanderbilt University, Nashville, TN 37204

Introduction

Recently, there has been a great interest in studying the interaction of strong time-dependent fields with atoms and molecules. This interest is largely motivated by advances in laser technology. In particular, there have been recent experiments with small hydrocarbon molecules subjected to short intense laser pulses.

Molecules exposed to strong laser irradiation get heavily ionized and undergo the Coulomb explosion. The Coulomb explosion is a process of rapid bond breaking and fragmentation of a molecule caused by strong Coulomb repulsion between the ions.



Computational Approach

- Density Functional Theory (DFT) is a well established approach that maps a complicated problem of N interacting particles onto a problem of N non-interacting fictitious particles.

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_n) \rightarrow n(\mathbf{r})$$

- Time-Dependent Density Functional Theory (TDDFT) is an extension of DFT to time domain, which allows to treat electronic excitations at reasonable computational cost.
- The motion of ions in our simulations is treated classically using quantum forces (Ehrenfest molecular dynamics).
- We studied the orientational dependence of fragmentation process by repeating the calculations for several representative configurations.

Computational Approach (cont.)

In this work, we study the ion dynamics in methane and ethylene subjected to 17 fs (FWHM) pulses of intensities of 8, 16, and 24 x 10^{14} W/cm^2.

Ethylene **Methane**

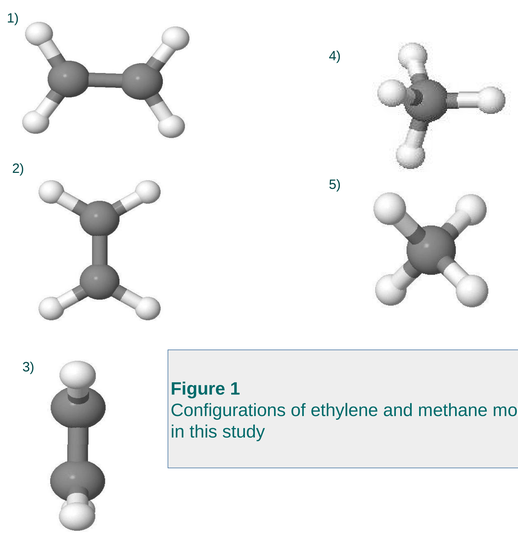


Figure 1
Configurations of ethylene and methane molecules in this study

Results

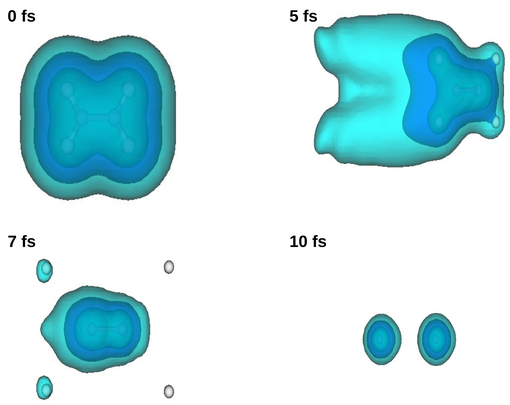


Figure 2
Electron density and ionic positions during the Coulomb explosion of C_2H_4

Results (cont.)

Ethylene **Methane**

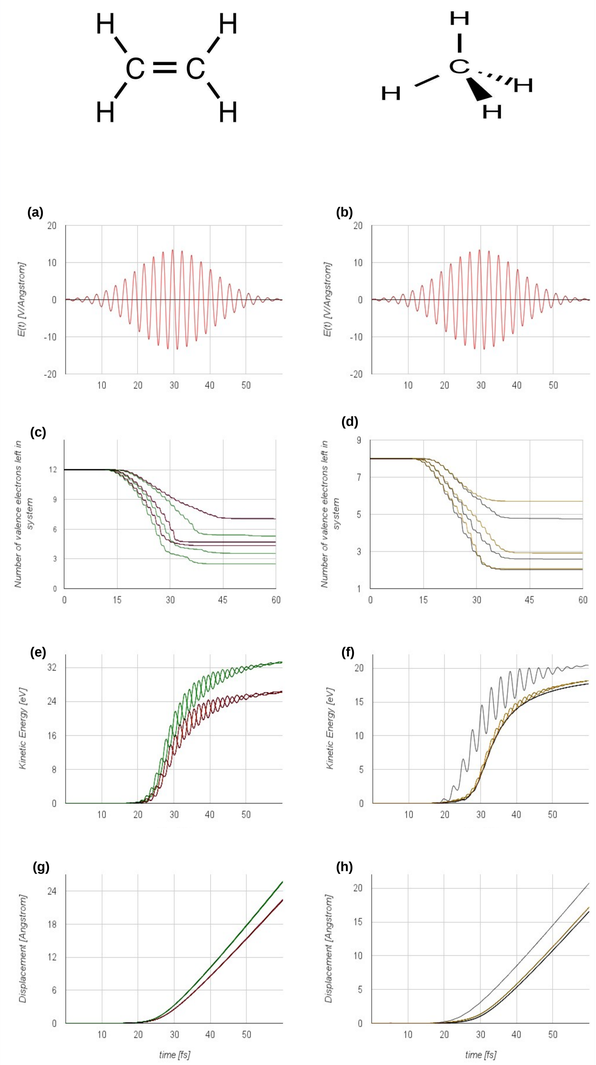


Figure 3
Ionization, kinetic energies of ions, and their displacements as a function of time. Green, red, blue, black and orange data corresponds to configurations 1, 2, 3, 4, and 5, respectively shown in Figure 1. (a), (b) Peak electric field magnitude of pulse at 24 x 10^{14} W/cm^2. (c), (d) Number of valence electrons left in the system. (e), (f) Kinetic energy of protons. (g), (h) Displacement of protons from their initial positions.

Summary

- We have shown that in the case of sufficiently high laser intensity the ejection of protons occur simultaneously, thereby confirming the all-at-once scenario proposed by Roither *et al*. [1] rather than the dynamic charge localization model by Markevitch *et al.* [2].
- We have found that for higher intensity pulses the kinetic energies of the protons ejected in each explosion are very similar in magnitude.
- Simulations show that the final ion energies are dependent on the orientation of molecules with respect to the laser polarization direction. However, the kinetic energies of all ions in a given explosion are very similar in magnitude.
- For the case of lower pulse intensity (8 x 10^{14} W/cm^2), the molecules undergo only partial fragmentation.

Literature cited

1. Roither, Stefan et al., Phys. Rev. Lett. **106**, 163001 (2011).
2. A. Markevitch et al., Phys. Rev. Lett. **92**, 063001 (2004)

Acknowledgements

I would like to thank Dr. Bubin, Dr. Varga, and everyone in the lab for the support.

I would also like to thank the ViNSE program for this opportunity, and the people who made this summer possible: Rene, Sarah, and Clare.

This work was supported by the NSF Grant: DMR-1005023