Comparison of ultrafast electron and X-ray diffraction - a computational study

Minas Stefanou, Kenichiro Saita, Dmitrii V. Shalashilin, Adam Kirrander

PII: S0009-2614(17)30219-1
DOI: http://dx.doi.org/10.1016/j.cplett.2017.03.007
Reference: CPLETT 34607

To appear in: *Chemical Physics Letters*

Please cite this article as: M. Stefanou, K. Saita, D.V. Shalashilin, A. Kirrander, Comparison of ultrafast electron and X-ray diffraction - a computational study, *Chemical Physics Letters* (2017), doi: http://dx.doi.org/10.1016/j.cplett.2017.03.007

Comparison of ultrafast electron and X-ray diffraction - a computational study

Minas Stefanou[a], Kenichiro Saita[a], Dmitrii V. Shalashilin[b], Adam Kirrander[a]

[a] *EaStCHEM, School of Chemistry, University of Edinburgh, David Brewster Road, Edinburgh EH9 3FJ, United Kingdom*
[b] *School of Chemistry, University of Leeds, Leeds LS2 9JT, United Kingdom*

Abstract

We compare ultrafast electron and X-ray diffraction using quantum molecular dynamics simulations in photoexcited ethylene. The simulations of ethylene are done using the *ab-initio* multiconfigurational Ehrenfest (AI-MCE) approach, with electronic structure calculations at the SA3-CASSCF(2,2)/cc-ppVDZ level. The diffraction signal is calculated using the independent atom model. We find that the electron diffraction is more sensitive the dynamics of the hydrogen atoms in the molecule.

Keywords: Quantum molecular dynamics, ultrafast electron diffraction, ultrafast X-ray scattering, ethylene, photochemistry

2010 MSC: 00-01, 99-00

1. Introduction

Ultrafast laser spectroscopy has developed dramatically over the past two decades, and constitutes today a large family of techniques capable of probing fundamental transformations of matter in astonishing detail [1, 2]. However, spectroscopy probes molecular rearrangements of geometry indirectly, in energy rather than in spatial coordinates, and inversion of the observed spectra often requires extensive high-level calculations. In contrast, diffraction probes molecular geometry directly. This key advantage was recognised by Ahmed Zewail, who even before his 1999 Nobel Prize was working

*Corresponding author
Email address: Adam.Kirrander@ed.ac.uk (Adam Kirrander)