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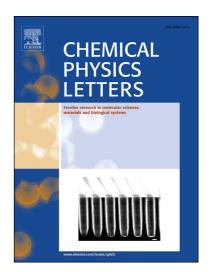
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ACCEPTED MANUSCRIPT

Ab-Initio Surface Hopping and Multiphoton Ionisation Study of the Photodissociation Dynamics of CS_2

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Abstract

New ab-initio surface hopping simulations of the excited state dynamics of CS_2 including spin-orbit coupling are compared to new experimental measurements using a multiphoton ionisation probe in a photoelectron spectroscopy experiment. The calculations highlight the importance of the triplet states even in the very early time dynamics of the dissociation process and allow us to unravel the signatures in the experimental spectrum, linking the observed changes to both electronic and nuclear degrees of freedom within the molecule.

Keywords: Photodissociation, Photoelectron spectroscopy, Theoretical Chemistry, Non-adiabatic dynamics

1. Introduction

- The dissociation dynamics of CS₂ following UV excitation have been
- a benchmark in chemical dynamics for many years, with numerous exper-
- 4 imental studies in both the time and frequency domain, see for example
- [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]. This lasting fascination with CS₂ can be traced

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