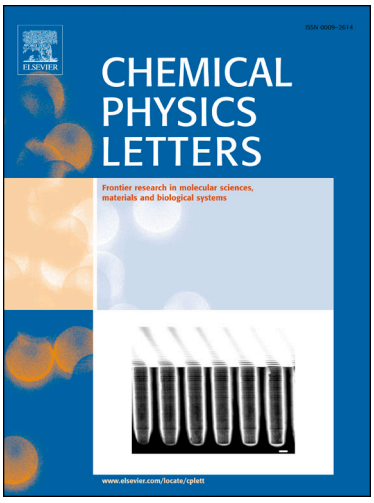

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Interference effects in electron scattering from small water clusters

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Abstract

The importance of interference effects in electron scattering from complex molecular targets is demonstrated theoretically by an exemplificative case study of small water clusters. Interference contributions arising from all the scattering centres in the target lead to an increase of the elastic differential cross sections at small scattering angles and to the appearance of prominent minima in the cross sections of three-dimensional isomers which resemble structural properties of bulk water. The phenomena which are absent for isolated water molecules but emerge for small water clusters may help to better understand electron-driven processes in condensed aqueous media.

Keywords: Electron scattering cross sections, Water clusters, Interference effects, Independent-atom model

1. Introduction

Collision processes involving water clusters, transient intermediates from gas phase to bulk water, are of paramount interest for radiation physics and chemistry [1–5]. Species consisting of a few tens or hundreds of molecules have been studied experimentally to explore important nanoscale processes of biological damage due to ionizing radiation [6–8]. It was shown that a water cluster environment can efficiently protect biomolecules against ionizing radiation [9, 10] or, in contrast, facilitate the production of secondary electrons and free radicals that react with the biomolecules [11–13].

Most experimental and theoretical studies performed to date have focused on the processes of electron attachment [14–17] and electron-induced fragmentation [7, 18] of water clusters. Knowledge and an accurate description of a broad range of electron-driven processes in aqueous environments are crucial for the understanding of the impact of radiation exposure on biological systems and for advancing the field of radiation therapy [19, 20].

Electron collisions with molecular clusters have been studied previously by means of standard *ab initio* techniques employing the coupled-cluster [21, 22] or the *R*-matrix [23] methods. However, as the system size increases, the computational complexity of these calculations increases significantly. Clusters composed of more than a few monomers are too big to be studied with the available *ab initio* computational implementations. In Refs. [24, 25], the multiple-scattering method [26] was applied for elastic scattering of low-energy (up to 10 eV) electrons from a $(H_2O)_2$

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