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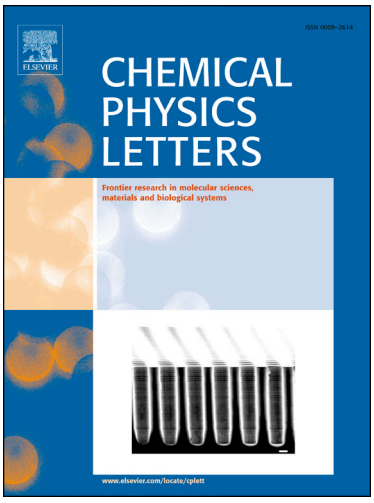

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Basis Sets for the Calculation of Core-Electron Binding Energies

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Abstract

Core-electron binding energies (CEBEs) computed within a Δself-consistent field approach require large basis sets to achieve convergence with respect to the basis set limit. It is shown that supplementing a basis set with basis functions from the corresponding basis set for the element with the next highest nuclear charge (Z+1) provides basis sets that give CEBEs close to the basis set limit. This simple procedure provides relatively small basis sets that are well suited for calculations where the description of a core-ionised state is important, such as time-dependent density functional theory calculations of X-ray emission spectroscopy.

Keywords: Core electron binding energies, basis set, x-ray photoelectron spectroscopy, density functional theory

1. Introduction

Calculations of core-electron spectroscopy have become increasingly important because of advances in X-ray light sources, such as free electron lasers. These sources can deliver short femtosecond pulses of X-rays which can probe ultrafast chemical processes [1–3]. One widely used technique is X-ray photoelectron spectroscopy (XPS) which involves the ionisation of core electrons. XPS is a powerful analytical tool that can provide information on elemental

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