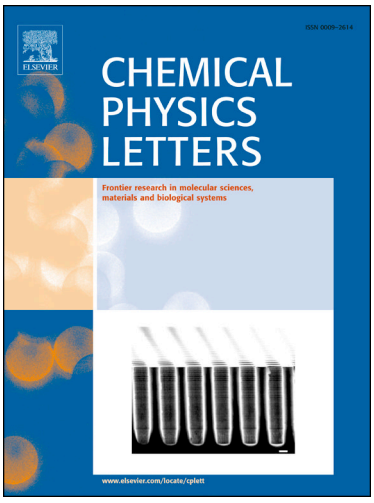

Frequency-dependent polarizabilities of diatomic molecules: density functional theory and *ab initio* methods compared with quantum-defect Green function technique

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Frequency-dependent polarizabilities of diatomic molecules: density functional theory and *ab initio* methods compared with quantum-defect Green function technique

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Abstract

The choice of optimal calculation method for frequency-dependent polarizabilities (FDPs) is important for many applications. We compare some density functional theory (DFT) and *ab initio* methods with the quantum defect theory (QDT). Since QDT incorporates the experimental energy spectrum, it should yield more reliable results for FDP near the resonances at the excited states. We show that the DFT and *ab initio* methods which demonstrate the best accuracy for the static polarizabilities, have poor accuracy of the excited states energies. Such a behavior is a source of some discrepancies between these methods and QDT technique.

Keywords: frequency-dependent polarizability, local-density functional, coupled cluster calculations, quantum-defect theory

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1. Introduction

Polarizability of atoms and molecules determine their most important electromagnetic properties, such as response to external electromagnetic field, van der Waals forces, polarization bremsstrahlung, *etc.* In the first nonvanishing

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