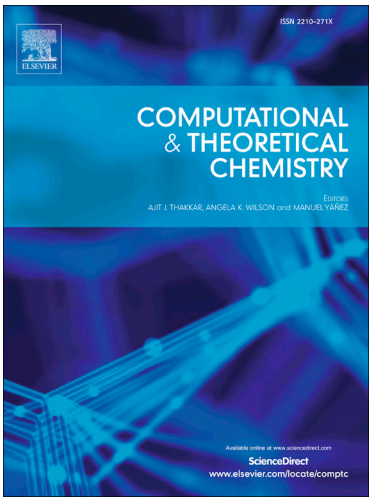

Interaction between 1-phenylethanone, 2-phenyl-2-propanol, and isopropenylbenzene with water molecules: A computational study

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Interaction between 1-phenylethanone, 2-phenyl-2-propanol, and isopropenylbenzene with water molecules: A computational study

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Keywords
Quantum chemical calculation, Molecular dynamics simulation, 1-Phenylethanone, 2-Phenyl-2-propanol, Isopropenylbenzene, Hydrogen bonding, Radial distribution function, Diffusion coefficient

Abstract

1-Phenylethanone, 2-phenyl-2-propanol, and isopropenylbenzene are representative molecules generated by the by-products of dicumyl peroxide remaining in cross-linked polyethylene. Although it has been reported that these molecules interact with water molecules and lower the electrical insulating ability of cross-linked polyethylene, the physicochemical details have not been clarified. In this study, the characteristics of the interaction between these molecules and water molecule(s) were evaluated using the quantum chemical calculations and molecular dynamics simulations. It was clarified that the interaction energy of 1-phenylethanone and 2-phenyl-2-propanol with water molecules is higher than that of the water dimer. On the other hand, the binding energy of isopropenylbenzene with water molecule is approximately one-half that of 1-phenylethanone-water and 2-phenyl-2-propanol-water. Furthermore, it was found that 1-phenylethanone and 2-phenyl-2-propanol reduce the diffusion coefficient of the water molecule. This promotes the formation of water clusters inside the insulating material and increases internal stress, which is one of the main causes of insulation degradation.

1 Introduction

Polymeric materials are used as electrical insulating materials in a wide range of electrical equipment, devices, and electrical power cables. In recent years, with the increased use of renewable energy sources, interest in solar power and wind power generation is gaining attention worldwide. For such power generation methods, long-distance power transmission is