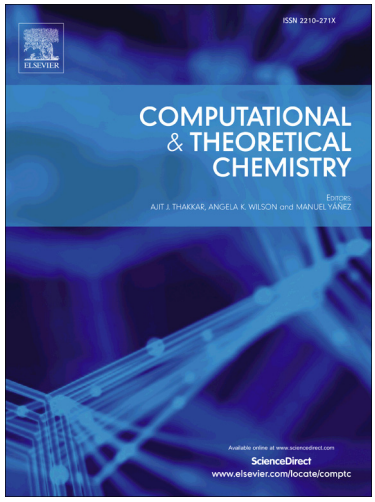

Theoretical Study of the Corrosion Protection Mechanism by Carbon Nanotubes

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Theoretical Study of the Corrosion Protection Mechanism by Carbon Nanotubes

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Abstract

The paint corrosion protection mechanism has been studied by density functional b3lyp/6-31GD3 (d, p) method using Gaussian09 program. The quantum-chemical study demonstrates the growth of anti-corrosion paint properties by the addition of carbon nanotubes (CNT) in the coating composition. Quantum chemical calculations have shown that the carbon nanotubes have a high affinity to the particles that support corrosion process (anions, oxygen molecules, hydroxyl groups). Thus, CNTs act as the adsorbents of micro particles that supports the corrosion process.

Keywords: carbon nanotubes, nanocomposite coatings, corrosion protection mechanism, quantum-chemical calculation

1. Introduction

The increase of the corrosion protection properties by using the coating with carbon nanotubes (CNT) as compared to the undoped material was established in a number of studies [1-8]. In [1], the hydrophobicity and anti-corrosion properties of the epoxy resin doped with carbon nanotubes (CNT) were studied. It has been shown that the CNT coating slows down the transport of water molecules to the substrate and enhances its protective properties. The USA Patent [2] shows that CNT can be effectively used to improve the mechanical properties of the epoxy composites and points to the possibility of creating the multifunctional epoxy composites with CNTs based on thermal and electrical properties of nanotubes. In [3-6], it was found that carbon nanotubes introduced in coatings increase the corrosion protection of steel and other materials. Authors [5,6] indicate that in many cases the CNTs act as a physical barrier to the corrosion process by filling in crevices, gaps, and micro holes on the surface of a deposit. Another reason for the decrease in the corrosion rate is the electrochemical mechanisms

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