

QM/MM methodology for studying the influence of ionic liquids in chemical reactions

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1. Introduction

Ionic liquids (IL), organic salts having a very low melting point draw scientific attention due to its structural diversity and physicochemical properties [1]. Initially, scientist concentrated on its bulk property but at present, the research advancements show that a better understanding of both bulk and atomic level nature are required to elucidate their full potential for various kinds of applications. The quantum mechanical theory (QM) is very accurate for such studies but is limited to small systems (1–10 nm), which only predict at the electronic level. However, molecular mechanics (MM) can efficiently work on macromolecular systems to predict the bulk properties but, it is not accurate. Hence, to identify the details of surface and interface properties of ionic liquids, a combined method is needed. The combined quantum-mechanical/molecular-mechanical (QM/MM) approach is a mostly accepted multiscale method that is suitable for studies involving both bulk properties and interactions at active sites inside IL bulk.

QM/MM method was initially established as a valuable tool for modeling large macromolecular systems especially bio/inorganic/organometallic systems. Warshel and Karplus first introduced this concept in 1972 in a study of the potential energy surfaces of the ground and excited states of conjugated molecules [2]. They approximated the σ -framework of the system using an empirical potential function and the π -electronic structure using the semi-empirical Pariser–Parr–Pople theory. This idea was also applied in the enzymatic reaction of lysozyme (carbocation stabilization in the active site) [3] by Warshel and Levitt in 1976. Hence, Warshel, Karplus, and Levitt were

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Chapter 12 - Polymers in robotics

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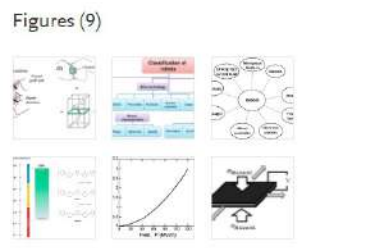
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Abstract

Robots and robotics are two familiar terms in the current era. The development of robotics was a milestone in technology and research. Artificial intelligence is key for the development of robotics. Nowadays, new inventions in robots and their applications are a hot topic. Polymers are an unavoidable part of robotics. The components of robots require a lightweight as well as durability and flexibility and, hence, polymers play an inevitable role. Thermoplastics, acrylates, urethanes, nanomaterials, etc., are being widely selected in robotics. Electroactive and conducting polymers are widely used classes of materials in robotics. The ionic and shape memory polymers also have an important place in robotics. Robots that are used to mimic living beings are an important part and are common in biological applications. They require flexible materials like polymers. This chapter provides a systematic analysis of different types of polymers used in the robotics field.

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