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Computational Chemistry Study of Propylene Polymerization on Ziegler—Natta Catalyst System

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Introduction

It is well known that polypropylene is one of the widely used polymeric materials. Actually, the world market for polypropylene is currently over 20×10^6 tons, and more than 80% of the global polymer is obtained with heterogeneous Ziegler-Natta catalysts. This work studies propylene polymerization on supported Ziegler-Natta catalysis system. Unfortunately, very little is known about the reaction itself because of difficulties with experimental studies of the catalytic system. The proposed calculations are aimed at providing a more detailed theoretical model of the catalyst. We calculated models of titanium catalysts and Ziegler-Natta catalytic systems, and also get the transition states. A better understanding of catalytic systems will lead to great practical advancements in the efficiency and economy of industrial polymerization processes.

Calculate Method

Quantum chemical molecular dynamics calculation of the propylene insertion reaction conditions and transition states during this reaction were carried out using Colors program developed in our laboratory [1]. It is based on the extended Huckel theory. Temperature was controlled by means of atom velocities. The calculations were performed for 5,000 steps with a time step of 0.1 fs at 343K. For comparison, density functional theory (DFT) method was also used for our calculation.

Result and Discussions

Before starting quantum chemical molecular dynamics (MD) calculation, the geometrical structures of the catalyst ($TiCl_3$-C_2H_5) and propylene as well as intermediates were optimized by Colors and ADF programs. Colors results were found to very similar to the results of ADF. Moreover the calculation using Colors program can be finished faster than the calculation by ADF. The transition states of propylene insertion reactions were calculated using our Colors program. Fig. 1 shows the model used for dynamics simulation, in which the reactant and surface were optimized respectively. Moreover the quantum chemical MD simulation was performed at the experimental temperature. The calculated results are in good agreement with the available experimental investigation.

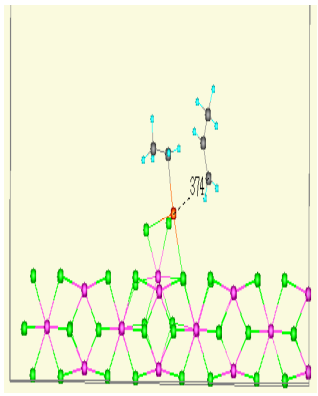

Fig. 1 shows the model used for dynamics simulation

Reference:

[1] T. Yokosuka et al., Jpn. J. Appl. Phys., 41 (2002) 2410.