

Stochastic simulations of polymer growth by Ni(II) and Pd(II) catalysts

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Abstract: Controlled design of polymer material with a specific microstructure is an emerging frontier in olefin polymerization. Recently, the hyperbranched polymers have been obtained with Pd-based diimine catalyst in ethylene polymerization under low pressure. Direct quantum chemical studies on the relationship between the catalyst structure, reaction conditions and the microstructure of a polymer are not practical without the aid of statistical methods. One such approach is a ‘mesoscopic’ scheme, in which the results of the density functional theory (DFT) based calculations are used as input data for a stochastic modeling of a polymer growth. In the present investigation we present examples of such a procedure. A model for performing stochastic simulations of polymer growth and branching has been developed and applied for the polymerisation processes catalyzed by the late-transition-metal-based catalysts. The results of the combined DFT/stochastic studies will be presented and compared with the available experimental data.

References:

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