

Methyl methacrylate reactivity under electric field in view of an electrically induced polymerization process

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We have studied the effect of a static external electric field on electronic properties of methyl methacrylate (MMA) and its consequences in an electro-initiated polymerization by density functional theory (DFT). The Conceptual-DFT scheme is used to obtain hardness (?), electrophilicity (?) and nucleophilicity (N) for MMA in gas phase and in a dielectric media. These changes on ? and N have been determined as a function of the direction and strength of the external electric field. This study give some insight on the enhancement of reactivity and, therefore, on the polymerization process under the presence of electric fields.