

## Explaining some anomalies in catalytic activity values in some zirconocene methyl cations: Local hyper-softness

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Some metallocene methyl cations made of zirconium, that have been used as catalysts in polymerization of ethylene, were studied by means of the conceptual density functional theory (DFT). Up to now, catalytic activity, a pure experimental parameter, that measures the kilograms of polyethylene produced per gram of metallocene, per time unit, per temperature unit, and per pressure unit, has been mainly explained in terms of steric hindrance at least qualitatively, meaning that a catalyst having a higher steric hindrance will present a lower catalytic activity. However, there has not been a satisfactory explanation for those few cases in which the steric effect cannot be linked with the catalytic activity, thus meaning that the electronic inductive effect predominates over the steric effect. As a consequence, the electronic inductive effect must be quantified through the use of a proper descriptor based on quantum chemical calculations and, in addition, this descriptor should be able to explain high values of catalytic activities even when the steric effect seems to play an unfavorable role. This work has demonstrated that a local reactivity descriptor called local hyper-softness coming from the conceptual DFT is a suitable pure theoretical parameter that explains such anomalies in some values of catalytic activity. It is expected that the findings exposed here can help to estimate catalytic activity and lead to a more rational design of new catalysts by means of computational chemistry. © 2013 American Chemical Society.