384e Confinement Effects on the Isomerization Kinetics of Small Hydrocarbons

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Nano-structured materials are frequently used to carry out chemical reactions due to their large surface area per unit mass and, in some cases, their potential for shape selectivity. It is, however, difficult to understand fully the role of the nano-structure in many chemical reactions due to the superposition of multiple effects. Such effects include: the reduced dimensionality of the system, the chemical heterogeneity of the pore surfaces, the possibility of selective adsorption of reactants/products, catalytic effects, and transport limitations. Experimental studies often show many of these effects at the same time, making the results difficult to interpret.

In this work we present results of *ab initio* calculations showing the effect of confinement in nano-porous carbons on the torsional potential and rotational isomerization rates for three four-membered hydrocarbons: butane, 1-butene and 1,3-butadiene. For these systems, we show how the reduced dimensionality of the pore space radically changes the potential energy surface and the reaction kinetics. These results are a first step towards an integrated model for the design of improved catalytic materials.