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The influence of overlap interactions on chemical reactions in confinement ERIK E. SANTISO, KEITH E. GUBBINS, Center for High Performance Simulation (CHiPS) and Department of Chemical and Biomolecular Engineering, North Carolina State University, AARON M. GEORGE, MARCO BUONGIORNO NARDELLI, Center for High Performance Simulation (CHiPS) and Department of Physics, North Carolina State University — Chemical reactions are often carried out in nano-structured materials due to their large surface area per unit mass. It is, however, difficult to understand fully the role of the nano-structure in many reactions due to the superposition of multiple effects. Such effects include: the reduced dimensionality of the system, the heterogeneity of the pore surfaces, the 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 density functional theory calculations illustrating the influence of overlap interactions (shape-catalytic effects) on chemical reactions. In particular, we show the effect of confinement in small pores on the rates of rotational isomerizations of n-butane, 1-butene and 1,3-butadiene. We find that the rates of these transitions change as the double exponential of the pore size in the molecular sieving limit. These results are a first step towards an integrated model for the design of catalytic materials.

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