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Computational Modeling and Advanced Synthesis Techniques for the Improved Design of ZSM-5 Zeolite Catalysts ARIAN GHORBANPOUR, JEFFREY RIMER, LARS GRABOW, University of Houston — Zeolites are the most widely used catalysts in industry. Active sites in zeolites are created by Al substitution of framework Si atoms in crystallographically different positions on the exterior or in the porous interior of zeolite crystals. This leads to heterogeneous chemical/kinetic behavior of various active sites, which can be employed to tune the properties of zeolites in catalytic processes. On the experimental side of this project, the shape selectivity of ZSM-5, an important zeolite catalyst in the petrochemical industry, is enhanced by manipulating its active site distribution. An advanced synthesis method was designed to passivate the external surface of ZSM-5 particles and suppress the reaction of bulky reactants over the exterior of the catalyst particles. The investigation of the impact of heterogeneous distribution of H-ZSM-5 active sites is continued through density functional theory (DFT) simulation, which reveals a large variation in the characteristics of 12 distinct active sites. The modeling of a test reaction indicates that pore confinement effects vary among different H-ZSM-5 active site locations, resulting in non-identical kinetic behavior through different extents of transition state stabilization. This heterogeneous performance not only causes different rates of reaction, but also impacts the dominant reaction mechanism at typical reaction conditions.

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