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MFI Zeolites with Substituted Heteroatoms for Selective Toluene Methylation

Ga/Fe-doped ZSM-5 variants that bias active sites to deliver >80% para-xylene selectivity for para-xylene production.

ZSM-5 zeolites are often used as catalysts for the conversion of toluene into valuable polymer precursors, such as para-xylene. However, the conversion of toluene into para-xylene can result in various undesirable side products being formed during the reaction, namely ortho-xylene and meta-xylene. Traditional methods only allow for a 30% yield of para-xylene, through either control of the thermodynamic equilibrium or via kinetics. One proposed approach towards increasing para-xylene selectivity has been through active site design, which would systematically bias sites towards smaller and straight sinusoidal channels. The use of structure-directing agents (SDAs) to position framework Al atoms and H+ sites towards smaller channel micropores has consequently led to an increase in para-xylene selectivity, using active site design methods. Nevertheless, the use of framework heteroatoms such as Ga, Fe, and B within ZSM-5 zeolites for para-xylene selectivity has been largely unexplored.

Purdue researchers have developed a variety of ZSM-5 zeolites utilizing heteroatoms such as Ga, Fe, and B due to their generation of H+ sites of differing acid strengths for the production of para-xylene. Catalysts were synthesized using either tetra-n-propylammonium (TPA) as the sole SDA or a mix of ethylenediamine (EDA) and TPA as co-SDAs. Researchers were able to demonstrate selectivity for para-xylene as the major product for the Fe and Ga catalysts when EDA and TPA were used as the co-SDAs. The selectivity for para-xylene was seen to be above 80% for the catalysts containing the co-SDAs, which is notably higher than the selectivity seen for the traditional TPA family (~30%). The developed catalysts show a superior control of both individual and total formation rates for para-xylene, translating into potential use in industrial and commercial applications.

Technology Validation:

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Chemicals & Advanced Materials/Specialty & Performance Chemicals
Chemicals & Advanced Materials/Polymer Science & Smart Materials
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-Powder X-ray diffraction patterns were taken of the synthesized zeolites to understand topology of the various heteroatom catalysts

-Elemental compositions of the samples were analyzed using inductively coupled plasma-optical emission spectroscopy

-Ar adsorption isotherms were used to determine micropore volumes

-First-order and zero-order rate constants for xylene formation were measured to understand individual and total product formation rates

Advantages:

-Higher selectivity for para-xylene compared to traditional catalysts

Applications:

-Para-xylene synthesis

TRL: 4

Intellectual Property:

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