Enhancing Zeolite Synthesis with Tailored Structure-Directing Agents (SDAs) and High-throughput Platform

by

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Abstract

The synthesis and applications of zeolites, porous materials with unique structures and properties, have been traditionally constrained by limited methodologies. The conventional techniques rely heavily on laborious trial-and-error processes, involving costly precursors and complex structure-directing agents (SDAs). This often leads to restricted catalyst selections and hinders the full utilization of zeolite's potential in various industrial applications. Addressing these challenges, this thesis presents an innovative, high-throughput platform for zeolite synthesis, offering a more efficient and versatile approach.

The platform's foundation is laid in the form of the Organic SDA Database (OSDB), a unique repository constructed using natural language processing and high-throughput binding energy calculations. The OSDB catalogs potential organic SDAs for targeted zeolite frameworks, providing a quantitative metric for comparing their effectiveness. It not only simplifies the SDA selection process but also expands the organic candidate pool, giving researchers better control over zeolites' physical and chemical properties.

Next, a high-throughput synthesis platform is introduced, designed to test multiple synthesis conditions simultaneously and optimize zeolite production. It vastly reduces the time and labor traditionally associated with zeolite synthesis, offering a practical solution to the laborious trial-and-error approaches of the past.

Following the establishment of the high-throughput platform, the thesis demonstrates its application by replacing conventional, costly, and complex organic SDAs with simpler and more economical ones. This innovative approach ensures the desired physicochemical properties of zeolites without compromising cost-effectiveness.

Additionally, the thesis explores the crystallization of a unique zeolite intergrowth using a single organic SDA. The successful synthesis of a tri-phasic zeolite intergrowth known as **MIT-2**, composed of **CHA**/**ERI**/**OFF** phases, underscores the versatility of the developed platform.

Finally, the methodology is extended to selectively crystallize specific zeolite phases from a multi-selective organic SDA. This process culminates in the synthesis of phasepure **LTA**-family zeolites, exhibiting the highest Si/Al ratios ever reported in hydroxide media. This achievement implies a significant improvement in zeolites' hydrothermal stability, potentially enhancing their catalytic lifetime and overall performance in targeted reactions.

In summary, this thesis offers an innovative, efficient, and versatile methodology for zeolite synthesis. The proposed high-throughput platform not only revolutionizes the traditional zeolite synthesis process but also opens up new avenues for catalyst selection. This advancement is poised to significantly contribute to the zeolite research field and broader society, by facilitating the design of custom zeolite catalysts for diverse industrial applications.

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