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Title: A Multi-scale Approach for the Discovery of Zeolites for Hydrogen Sulfide Removal

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ACCEPTED MANUSCRIPT

- Discovery of zeolites with reverse adsorption selectivities for H2S removal
- Detailed process modeling and optimization for adsorption-based H2S removal
- Identified the most cost-effective zeolites for H2S removal using PSA
- Minimized total investment and operating costs.
- Novel use of shape-, pore- and size-selectivities for zeolite screening

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