Spiral Feedback for Catalyst Design: Experiment and Theory

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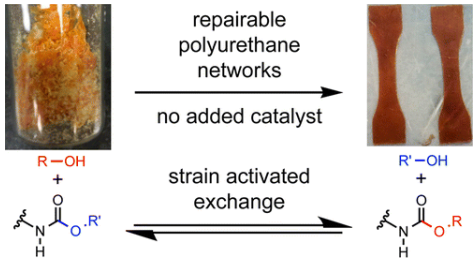
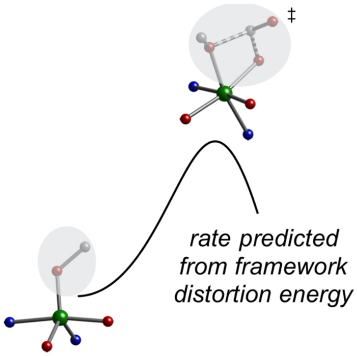
Abstract

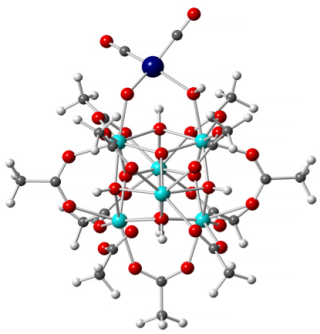
The ideal partnership of theory and experiment finds them employed concomitantly, with available experimental results serving to validate a theoretical model, theory being used to rationalize variations in experimental observables as a function of alternative conditions or variables, and theory ultimately being employed a priori to streamline the design of improved, next-generation systems having improved properties or characteristics. In the case of catalysis, the relevant properties tend to be activity and selectivity, to name two.





In collaboration with experimental groups in the NSF-funded Center for Sustainable Polymers and the DOE-funded Inorganometallic Catalyst Design Center, my theoretical research group has been focusing on a wide variety of catalytic processes, including vitrimer repair/relaxation, ring-opening transesterification polymerization (ROTEP) of cyclic esters, and exploitation of shale-gas products employing metal-organic-framework (MOF) nodes as catalytic supports for well defined transition-metal catalysts. I will describe our recent progress in all three of these areas, paying special attention to the critical interplay of theory and experiment as it has fostered progress. Remaining challenges and opportunities for theory in particular will be highlighted.

References



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