

***Towards a “Greener” Route for
Acetic Acid Production via the
Carbonylation of Dimethyl Ether
Over Small-Pore Molecular Sieves***

**Monday
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3:00 pm
Wu and Chen Auditorium
Levine Hall**



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Abstract

Catalyst design is a critical pillar, and current bottleneck, in the construction of a sustainable chemical industry. Practical catalytic materials are earth-abundant, active, selective, and stable. Developing materials that meet these criteria is challenging and involves a two-phase process that (1) extracts molecular-level understanding of the origin of reactivity for a given chemical pathway, and (2) exploits this understanding through tailored synthetic techniques.

In this talk, I will focus on catalyst design for the Koch-type carbonylation pathway, a reaction that is of practical interest since it provides a rare noble metal- and halide-free route to producing an important chemical intermediate, acetic acid. I will present the characterization of the reactivity of the small-pore molecular sieve with the chabazite structure for this reaction. From the analysis of materials synthesized with different active site densities and strengths, in conjunction with theoretical investigations, we obtain fundamental insights into the descriptors of reactivity for the carbonylation reaction in this small-pore material. These insights, in turn, can be used to intelligently direct the investigation of other small-pore molecular sieves with tuned confining environments and chemical compositions, and motivate the development of synthetic techniques that control active site distributions in a broader range of solid materials. Collectively, our studies provide a successful example of the first step in the process of tailoring catalytic materials for new applications through rational design methods.

Bio

Marcella Lusardi is a postdoctoral scholar at Caltech, working with Professor Mark E. Davis. Her research interests are in the synthesis and design of new heterogeneous and photo- catalytic materials for green chemistry applications. Dr. Lusardi received her PhD at MIT with Professor Klavs F. Jensen in Materials Science and Engineering in 2018. Prior to that, she graduated from Columbia University with a B.S. in Chemical Engineering in 2012.

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