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SEMINAR SERIES

HIGHLIGHTS IN ENERGY RESEARCH

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Sipping from the Holy Grail: Simulating the Self Assembly of Nanoporous Materials

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Zeolites are the most used catalysts by weight on earth and offer the potential for new applications in carbon dioxide capture, biofuel production, and nano-electronics. The applications of zeolites arise from their nanoporous crystalline structures and stabilities. Despite the great importance of zeolites, zeolite chemists still rely heavily on trial-and-error in their search for new materials, because the mechanisms controlling zeolite formation remain poorly known. Understanding such mechanisms will be critical to one of the "holy grails" of materials science -- rational design of tailor-made nanoporous materials. In this lecture, we tell the story of a multi-scale molecular modeling programme [1] in search of this holy grail.

We begin by reviewing present-day understanding of zeolite synthesis with a focus on the role of "structure directing agents" (SDAs). We study this problem through a multi-scale application of Density Functional Theory (DFT) and Monte Carlo (MC) methods. Our DFT calculations provide key structural and energetic parameters, and explain the curiously wide range of bulk moduli observed for silica polymorphs. We then discuss models of silica polymerization sampled with MC to simulate amorphous silica, silica-SDA nanoparticles, zeolites, and mesoporous silica. Our MC simulations reproduce NMR signatures of silica polymerization; predict that such polymerization is not diffusion controlled; and reveal sought-after structures of silica-SDA nanoparticles. Replica exchange MC is found to be essential for modeling zeolite crystallization, allowing predictions of SDA sizes that optimize zeolite yield and crystallization rate. We conclude with remarks about the potential for molecular modeling to peer even more deeply into the atomic dance of nanopore formation.

[1] SM Auerbach, W Fan, and PA Monson, "Modeling the Assembly of Nanoporous Silica Materials", International Reviews in Physical Chemistry **34**, 35-70 (2015). (https://doi.org/10.1080/0144235X.2014.988038)

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Dr. Scott Auerbach is full professor of physical and computational chemistry at the University of Massachusetts Amherst. Professor Auerbach's research focuses on modeling the behavior and self-assembly of nanostructured materials and catalysts such as zeolites – of importance to emerging renewable energy technologies including biofuels and fuel cells – leading to 2 books and over 110 peer-reviewed articles. Professor Auerbach graduated with a BS in Chemistry from Georgetown University in 1988; and with a PhD in theoretical chemistry from UC Berkeley in 1993. After an NSF-funded postdoc at UC Santa Barbara, Dr. Auerbach began his academic position in 1995 at UMass Chemistry, and was promoted to full professor in 2004. Professor Auerbach has won several research awards including an NSF Career Award in 1998, a Sloan Fellowship in 1999, and a Camille Dreyfus Teacher-Scholar Award in 1999.