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

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Abstract: Zeolites are the most used catalysts by weight on earth [1] and offer the potential for 21st-century applications in carbon dioxide capture, biofuel production, and nano-electronics. The present and future applications of zeolites arise from their nanoporous crystalline structures, and from their impressive 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 [2] 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 then review other modeling efforts to shed light on zeolite synthesis, concluding that there is need for physically-based algorithms for constructing zeolites capable of reaching relevant length and time scales. We fill this need 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 coarse-grained models of silica polymerization sampled with MC to simulate the formation of 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] "Handbook of Zeolite Science and Technology," Eds. SM Auerbach, KA Carrado, PK Dutta, New York: Dekker, 2003.

[2] 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)

Bio: 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 and a minor in Mathematics 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 Camile Dreyfus Teacher-Scholar Award in 1999. From 2008-2016, Prof. Auerbach was the founding director of the Integrated Concentration in Science (iCons) Program at UMass, which challenges undergraduate science and engineering students to integrate fields of study to design solutions for societal problems in renewable energy and biomedicine. In 2016, Prof. Auerbach won the inaugural UMass Manning Prize for Teaching Excellence on the Amherst campus; and in 2017 Auerbach won the UMass Distinguished Teaching Award, the highest teaching honor at UMass Amherst.