

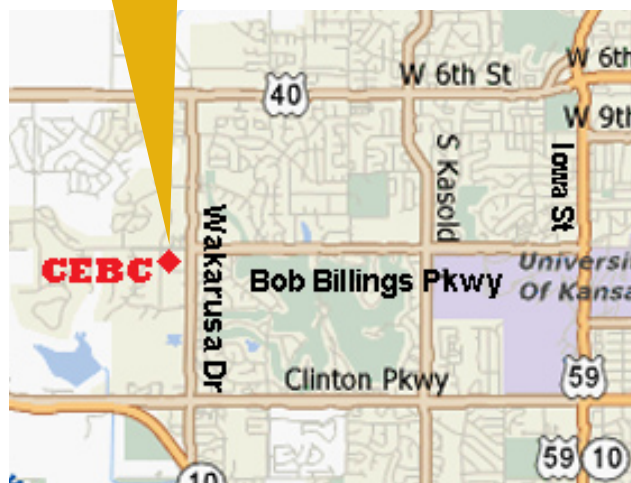
New Nanoporous Materials for Practical Applications Using Computational Modeling

How Close Is the Dream to Reality?

Nanoporous materials such as zeolite or metal-organic frameworks have many potential applications, including as adsorbents and active components in membranes for chemical separations. The ability to use computational modeling in a genuinely predictive way to develop new nanoporous materials for targeted applications has been a long standing goal (dream?) in the research community. I will talk about how recent advances are bringing this goal within reach and what opportunities and barriers exist with these approaches in the future.

**9:00 a.m. Tuesday
September 19, 2017**

CEBC Seminar Room, B104
Building B, 1501 Wakarusa Drive,
Lawrence, KS



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About the presenter

Professor David Sholl's research uses computational materials modeling to accelerate development of new materials for energy-related applications, including generation and storage of gaseous and liquid fuels and chemicals and carbon dioxide mitigation. He has published over 300 papers. He has also written a textbook on Density Functional Theory, a quantum chemistry method that is widely applied through the physical sciences and engineering. David is a Senior Editor of the ACS journal Langmuir. More information on David's research group is available from www.chbe.gatech.edu/sholl

The Center for Environmentally Beneficial Catalysis (CEBC) at the University of Kansas and its partners are developing green technologies to help the chemical industry prevent waste and conserve the earth's natural resources.

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