Expanding the chemical palette for reliable adsorption-based separations

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Abstract: The majority of research literature on chemical separations focuses on a relatively small collection of chemicals. In many ways this is appropriate because of the dramatic economic and environmental impacts of these species. The space of possible chemicals, however is vast; Carl Sagan's famous "billions and billions" is many orders of magnitude too small for chemical space. I will discuss early steps towards methods that may eventually allow rapid development of adsorbent-based separations for a diverse range of molecules drawn from a broad chemical space. I will also discuss recent attempts to quantify reproducibility of experimental data in adsorption, a topic that brings up wide-ranging issues in forming connections between basic discovery-oriented science and the practical application of materials in real-world separations.

Biography: David Sholl is the John F. Brock III School Chair of Chemical & Biomolecular Engineering at Georgia Tech. David'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 carbon dioxide mitigation. He has published over 300 papers that have received over 13,000 citations. 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 and he was instrumental in the development of RAPID, a $70M DOE-funded Manufacturing Institute focused on process intensification run by AIChE. More information on David's research group is available from sholl.chbe.gatech.edu

When: Tuesday, March 27, 2018 at 4 pm
Where: EP#252