**Compositional and structural order at inorganic-organic interfaces**

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Advances in synthesis and characterization capabilities enable the atomic-scale features and properties of engineering materials to be measured, understood, and controlled in ways that have not previously been possible. Technologically important examples include heterogeneous catalysts, such as nanoporous aluminosilicate zeolites and mesoporous nitrogen-containing carbons, whose hydrocarbon conversion and electrocatalyst properties have been challenging to understand and control. This has been due in part to their non-stoichiometric compositions, semi-crystallinity, and heterogeneous surfaces, which result in complicated compositional and structural order and disorder that have important influences on their adsorption and reaction behaviors. Intriguingly, many key features appear to arise due to strong interactions between a crystallizing network and specific ion species in solutions or melts.

By using a combination of X-ray diffraction, solid-state nuclear magnetic resonance (NMR) spectroscopy, electron microscopy, molecular modeling, and bulk property analyses, such materials can be probed over multiple length scales to obtain and correlate insights on local bonding environments and interactions with macroscopic catalytic properties. Recent results will be presented on understanding catalyst compositions and structures at an atomic level. In particular, I will highlight opportunities where insights from spectroscopic and molecular modeling analyses might be combined to establish the molecular interactions that lead to crystalline order or account for distributions of surface active sites. The analyses provide guidance for the rational design and engineering of catalysts for hydrocarbon conversion, pollution mitigation, and electrochemical device applications.