

Identifying New Paradigms in Crystal Engineering for Catalysis and Biomedical Applications

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Crystal engineering is a broad area of research that focuses on methods of designing and/or optimizing materials for diverse applications in fields spanning energy to medicine. The ability to selectively control crystallization to achieve desired physicochemical properties requires detailed understandings of the thermodynamic and kinetic factors regulating crystal nucleation and growth. Combining this fundamental knowledge with innovative approaches to tailor crystal size, structure, and morphology has the capability of producing materials with superior properties beyond what is achievable by conventional routes. In this talk I will discuss two general mechanisms of crystal growth: (1) classical pathways involving 2-dimensional layer nucleation and advancement on crystal surfaces through monomer addition; and (2) nonclassical pathways, termed *crystallization by particle attachment* (CPA), involving the formation of metastable precursors that play a direct role in crystal nucleation and growth. Our group uses atomic force microscopy (AFM) to monitor crystallization, and we have developed advanced AFM techniques to elucidate CPA processes *in situ* under solvothermal conditions. This unique AFM system is capable of capturing time-resolved dynamics of particle addition and post-attachment rearrangement, thus opening new pathways to probe crystal growth at realistic synthesis conditions. We also design “modifiers” to control crystal properties such as size and morphology. Modifiers are molecules or macromolecules that interact with specific surfaces of crystals and regulate anisotropic growth rates. In this talk, I will show how we use growth modifiers to control crystallization in two distinctly different, yet fundamentally similar research areas. In the first part of my talk, I will discuss our work on the development of therapeutic drugs for crystals implicated in both pathological and infectious human diseases – notably kidney stones (calcium oxalate monohydrate) and malaria (hematin). In the second part of my talk, I will discuss how we are using modifiers as a bio-inspired approach to tailor the properties of zeolites, which are microporous materials employed commercially in catalysis, adsorption, and ion-exchange processes. Our group uses zeolite growth modifiers (ZGMs) to tune crystal properties. I will discuss how we select ZGMs and characterize their efficacy using techniques that probe macroscopic to molecular length scales. I will also address broader challenges of synthesizing zeolites and introduce the unique ways in which we are investigating their mechanism(s) of growth and developing commercially-viable approaches to control their chemical composition.