Nanostructure Inorganic-Organic Hybrids:
Engineering a New Class of Porous Materials

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Porous materials play a crucial role in many important applications including air purification, gas separations, catalytic processes, and chemical sensing. The design of materials for such applications requires a fundamental understanding of the adsorption and reactivity between target molecules and high surface area nanomaterials, but serious gaps exist in this area. Metal sites in zeolites and impregnated carbons are known to give rise to special adsorption and catalytic behavior. However, tailoring these materials for specific interaction with adsorbate molecules is limited by the inherent disorder of such sites, large pore size distributions, and rigid structures that are not amenable to chemical modification.

Metal-organic frameworks represent a new direction in porous materials research that could lead to the creation of designer-specific multifunctional materials. The rich field of coordination chemistry provides a versatile platform from which these materials may be assembled from an almost infinite set of building blocks. These new inorganic-organic hybrid materials are formed through interconnection of metal clusters and organic ligands. They have demonstrated interesting adsorption properties and have a clear potential for impacting a wide range of adsorption-based technologies.

Understanding the adsorption and catalytic properties of MOFs will help narrow down the design scope and facilitate the development of functional materials to perform targeted separations and purifications. In this presentation, this new class of materials will be introduced and current research in this emerging area will be discussed. Adsorption experiments and molecular modeling results will be presented for several gases on model MOFs. Specific discussion will be given regarding the effect of pore size, unsaturated metal sites, and functionalized ligands on the adsorption of light gases. The implications of these results for impacting adsorption applications such as separations, catalysis, and controlled storage and release will be discussed.