612g Theory and Computer Simulation of Adsorption in Templated Molecular Recognition Materials

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Molecular recognition is a process of strong and specific binding between a molecule and a substrate. This mechanism plays a vital part in many biological processes, including enzyme function, genetic information replication, antibody-antigen interactions, etc. One of the major material engineering efforts over the last two decades has been to translate this mechanism to synthetic templated molecular recognition (TMR) materials for adsorption, separation, catalysis, sensing, protein immobilization and other applications. The design of these materials requires a molecular understanding of the templating effect on material structure and performance. In this work, we present a theoretical description of adsorption in a model templated porous material.

Our model material is a quenched, equilibrated mixture of template and matrix molecular species where the template component has been subsequently removed. We propose a set of site-site (i.e. RISM) replica Ornstein-Zernike equations, relating the correlation functions of template, matrix, and adsorbing fluid molecules. We explore adsorption in systems templated with structurally and energetically heterogeneous species and outline, for the first time, the minimal model featuring molecular recognition effects. We verify these effects by grand canonical Monte Carlo simulation and discuss their implication to the design of templated molecular recognition materials.