

## Confinement of Organic Molecules in Nanoporous Minerals

DI WU<sup>1</sup>, HUI SUN<sup>1,2</sup>, XIAOFENG GUO<sup>1</sup>  
AND ALEXANDRA NAVROTSKY<sup>1</sup>

<sup>1</sup>Peter A. Rock Thermochemistry Laboratory and  
Nanomaterials in the Environment, Agriculture, and  
Technology Organized Research Unit (NEAT ORU),  
University of California, Davis, One Shields Avenue,  
Davis, CA, 95616, USA

<sup>2</sup>State Key Laboratory of Chemical Engineering, East China  
University of Science and Technology, Shanghai, 200237,  
China

Confinement of organics in nanoporous inorganic media is a very important topic in various research fields, including biomineralization, geological carbon sequestration, industrial catalysis and medicine. In order to reveal insights into organic-mineral interactions in pores, we have performed systematic studies of the thermodynamics, structures, and dynamics on confinement of various organic guests (quaternary ammonium ions, amines and alcohols, hexane and several organic solvents) in zeolites and mesoporous silicas (0.4 to 20.0 nm pores). We employed different calorimetric techniques to investigate the enthalpies of interaction between the hosts and guests. We also monitored the interactions using XRD, IR, TG-DSC and solid state NMR. Our studies reveal that the enthalpies of interaction range from a few kJ to as much as -200 kJ per mole of organic. The magnitude of the interaction energy is governed by the dimensions and surface properties of the inorganic hosts as well as the structure, phase and dynamics of confined organic guests. Three types of inclusion were documented, single-molecule confinement, multi-molecule adsorption/confinement and nanocrystal confinement. Our studies provide comprehensive information describing organic matter-mineral interactions in various conditions.