Mesoscale Priority Research Direction

Role of Solvent Meso-Structures in Catalysis

Opportunity

Water will 'self-organize' around small molecules e.g. H_2, methane, CO_2 to make crystalline clathrate hydrates.[a] Organization of water around protein molecules affects binding, recognition and enzyme catalysis.[b] Local solvent organization must play a role in nonenzymatic catalysis but *there is no systematic understanding of how or when.*

This opens opportunities for new approaches to promote and control chemical transformations.

Approach

***Structural probes* e.g. neutron scattering will identify patterns of local static and time-average departures from bulk liquid structures. *Modeling* will provide thermodynamic parameters for representative organization patterns, and a language for their description. *Experiment* will test this language, and identify new catalysts to take advantage of organization-driven rate enhancements.**

Meso Challenge

How do we develop a systematic description of local solvent organization? How do we predict when one hypothetical transition state will be stabilized by solvent organization whereas another will be destabilized – and intentionally design catalyst bodies accordingly?

Impact

It has already been demonstrated that intentional encapsulation of catalysts has dramatic effects on reaction rates.[c] By developing and exploiting a systematic understanding of solvent organization we will enable more general control of reaction selectivities and rates.

References: a) Lokshin et al, Phys. Rev. Lett 2004, 93, 125503-1 b) Snyder et al, Proc. Nat. Acad. Sci. USA 2011,108, 17889
c) Pluth et al, Science 2007, 316, 85

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