the level/magnitude necessary.

This has been talked about for some time, but not done at

in molecular computational/reaction network models.

real catalytic systems to help validate and tune parameters

Proposed Solution: Combine the two, using data from

be an accurate representation of the real system

(2) need to a priori define model, which may or may not

models, but they are limited by (1) inherent accuracy and

individually reaction steps and developing complex reaction

Molecular computations are powerful ways of isolating

complex—Grand Challenge: "in situ methods."

Real catalysts and catalytic processes are extremely

Research: Catalysts that Function at the Nanoscale; June 19-20, 2003

Bemhard L. Troup, Dep't of Chem. Eng., MIT; NSF "Future Directions in Catalysts

and Molecular Computational Methods

Need for Careful Integration of Experimental