Need for Careful Integration of Experimental and Molecular Computational Methods

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- **Real catalysts** and catalytic processes are extremely complex– Grand Challenge: "*in situ* methods."
- **Molecular computations** are powerful ways of isolating individual reaction steps and developing complex reaction models; but, they are limited by (1) inherent accuracy and (2) need to *a priori* define model, which may or may not be an accurate representation of the real system
- **Proposed Solution**: Combine the two, using data from real catalytic systems to help validate and tune parameters in molecular computational/reaction network models. This has been talked about for some time, but not done at the level/magnitude necessary.