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**Quantitative Assessment of Channeling Mechanisms in Nanoscale Catalytic Architectures**

Our research group is focused on materials for electrocatalysis, particularly non-precious electrocatalysts for fuel cell reactions. We approach this challenge in two ways: using transition metal catalyst centers and redox enzymes. These approaches are similar in that catalytic turnover is much lower than precious metal catalysts such as platinum, and transport in electrode layers becomes important when catalyst loadings are increased to compensate for low activity.

Natural and technological instances of enzyme catalysis often feature multistep reaction cascades. The throughput and yield of such nanoscale catalytic architectures is limited by the ability to retain reaction intermediates and direct them toward downstream reaction steps. Nature has settled on several approaches to intermediate channelling, including electrostatic attraction, confinement, and surface affinity. This presentation will discuss the limits of such approaches through modeling, from the molecular dynamics to continuum scales. Geometric factors are considered at the continuum scale, where electrostatic interactions are shown to be much more effective than proximity alone. Short range molecular interactions are also significant, however, and molecular dynamics studies will demonstrate structures that we have found to yield high catalytic efficiency. Molecular-scale results can be combined in a Kinetic Monte Carlo model that can be compared directly to experiment.