

# Theoretical Physical Chemistry Seminar



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4:00 PM

Zoom

## “Harnessing Conformational Dynamics to Engineer New Enzymes”

Understanding how new enzyme functions evolve, either on existing scaffolds, or completely *de novo* on previously non-catalytic scaffolds, is of great interest both from a fundamental biochemistry perspective, and from a biotechnological perspective. Several hypotheses have been put forward to rationalize enzyme evolution, one of which is that their conformational dynamics plays an important role in facilitating the emergence of new enzyme functions. My team and I have invested substantial research effort into understanding enzyme multifunctionality in catalytically promiscuous enzymes, as well as the structure-function-dynamics relationships shaping the evolution of new enzyme functions, in both natural and engineered active sites. In this talk, I will discuss recent progress in this area, and illustrate how we have engineered conformational dynamics to generate a *de novo* active site capable of catalyzing a non-natural reaction, and then subsequently enhanced this activity using a simple computational approach, reaching catalytic efficiency comparable to that of naturally occurring enzymes.