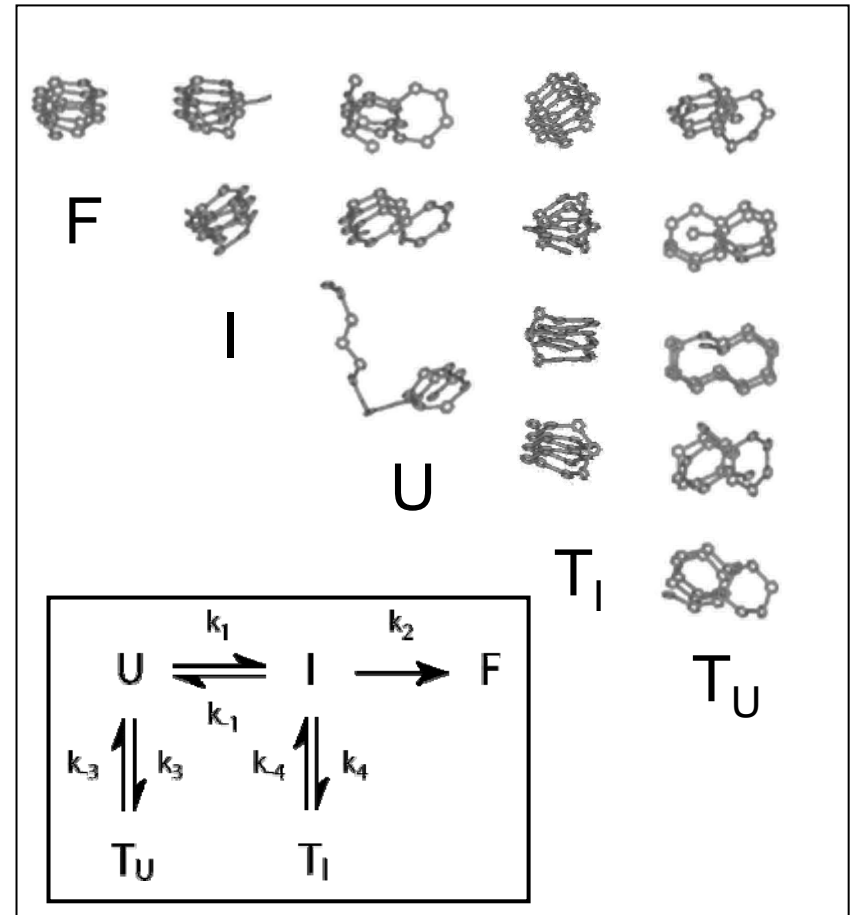


Simulations of polyphenylacetylene (PPA) “foldamers”

Vijay S. Pande, Stanford University

- **What are PPA “foldamers”**
 - nonbiological polymers that fold
 - model systems for self-assembling nano structures
 - challenge for simulation: long timescale and complex dynamics
- **New results**
 - longer chains considerably are more complex: multiple traps and remarkable complexity
 - new methods used to predicted long timescale behavior: Markovian model and Folding@Home grid computing
 - Folding@Home: a new paradigm of combined research and outreach



Work performed by Sidney Elmer, CPIMA supported graduate student