OpenPath Sampling

Features

Methods implemented:

- Transition Path Sampling
- Transition Interface Sampling
- Replica Exchange TIS
- Multiple State TIS
- Multiple Interface Set TIS
- Single Replica TIS
- Adaptive Multiple Splitting
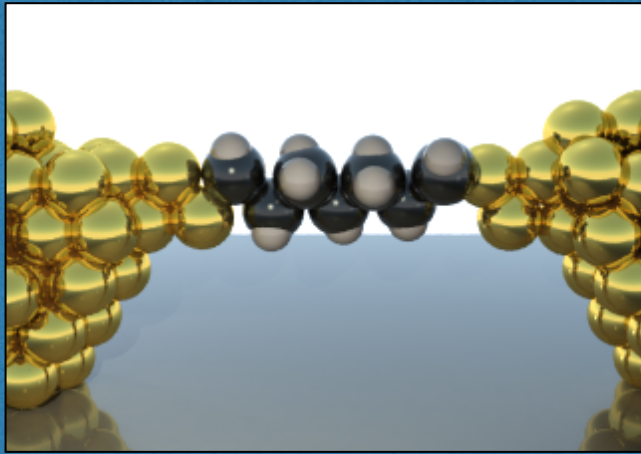- Forward Flux Sampling

Version 1.0: coming soon!

Additional features coming
late spring/early summer

Engines supported:

- Toy Dynamics
- OpenMM
- LAMMPS
- Generic external engine

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New approaches mapping second quantization to classical variables make it possible to explore previously inaccessible topics in chemical physics

A new and efficient algorithm for SC-IVR calculations provides a faster way to calculate quantum correlation functions including dynamical interference effects
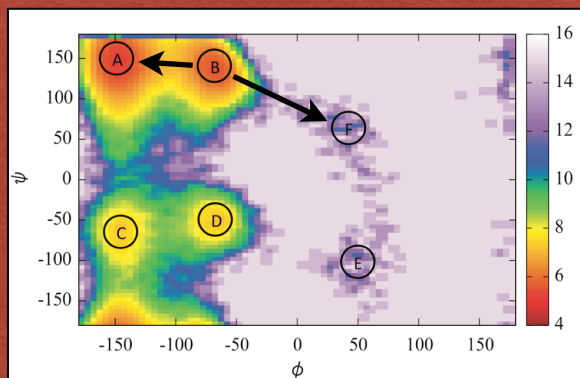
Rare events methods enable simulations of important transitions in problems ranging from biology to materials science