

Path sampling and the OpenPathSampling LAMMPS interface

David W.H. SWENSON (University of Amsterdam)

Path sampling methods, such as transition path sampling (TPS) and transition interface sampling (TIS), are powerful methods for studying rare but important events in complex molecular systems.

This talk will present the methodology of path sampling, as well as an example of its use to study the underlying differences in dynamics between a wild-type and oncogenic mutant protein, explaining why the mutant causes cancer.

Finally, the OpenPathSampling software package will be introduced, including its preliminary interface with LAMMPS.