Clotilde FERMANIAN

Université de Paris 12.

Single switch surface hopping for molecular dynamics

In this talk, we present a trajectory surface hopping algorithm solving non adiabatic transitions. This algorithm is called "single switch surface hopping" because non adiabatic transitions are only performed when a classical trajectory attains one of its minimal surface gaps. It stems from a mathematically rigourous analysis of propagation through conical intersections. We will discuss the convergence and the convegence rate of the algorithm for two-modes Jahn-Teller systems and present its generalization to three-modes pseudo Jahn-Teller models.