

### **Prerequisites:**

- Introduction of generalized coordinates
- KE operator in Lagrange form
- Smooth approximations of PES and IDS

### **Individual trajectory:**

- Initial condition generation
- Classical trajectory propagation
- FT of dipole time-dependence

### **CIA spectra from trajectory ensemble:**

- Spectral function as ensemble average
- Desymmetrized CIA spectral profile

2-5 mln. trajectories

