# Nonadiabatic EXcited state Molecular Dynamics (NEXMD) code

CyberTraining 2021 Workshop

Walter Malone
Los Alamos National Laboratory
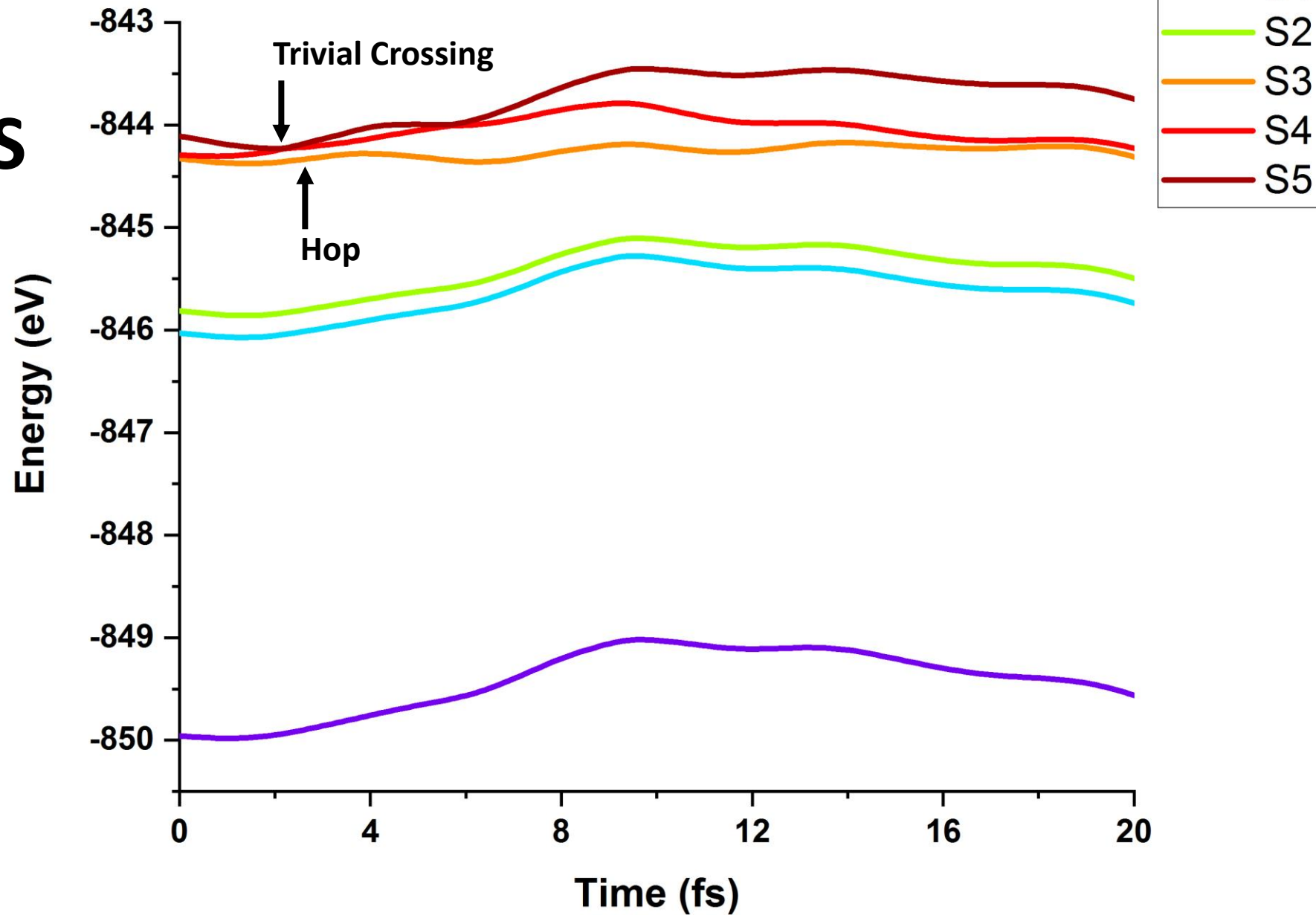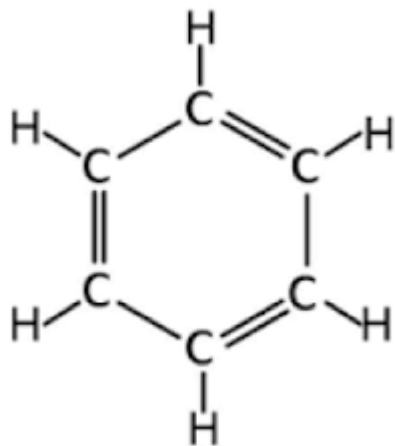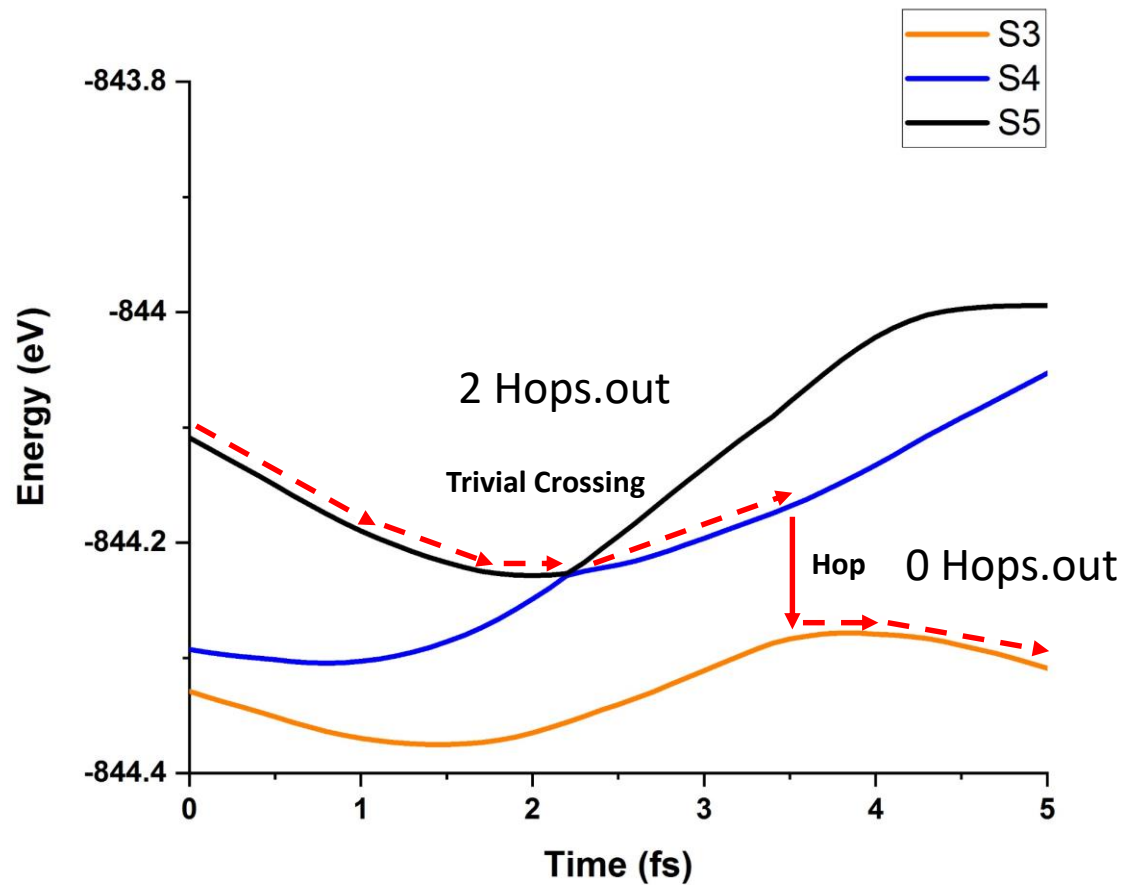
# Outline

- Introduction and Compilation
- Base Functions
  - SCF convergence
  - Geometry optimization
  - Excited state structure
    - CIS vs RPA
  - Excited state optimization
  - Adiabatic dynamics in ground and S1 state
    - Newtonian Dynamics vs Langevin Dynamics
  - Dynamics in the present of solvent
    - Linear response vs Vertical excitation vs State-specific
- Nonadiabatic Dynamics
  - Single Trajectory
    - Decoherence, surface hopping dynamics
  - Ground State Trajectory
  - Single Point Calculation Setup
  - Generating an Optical Spectrum
  - Setting Up and Running a Swarm of Trajectories
  - Analysis
- Bonus Development Features
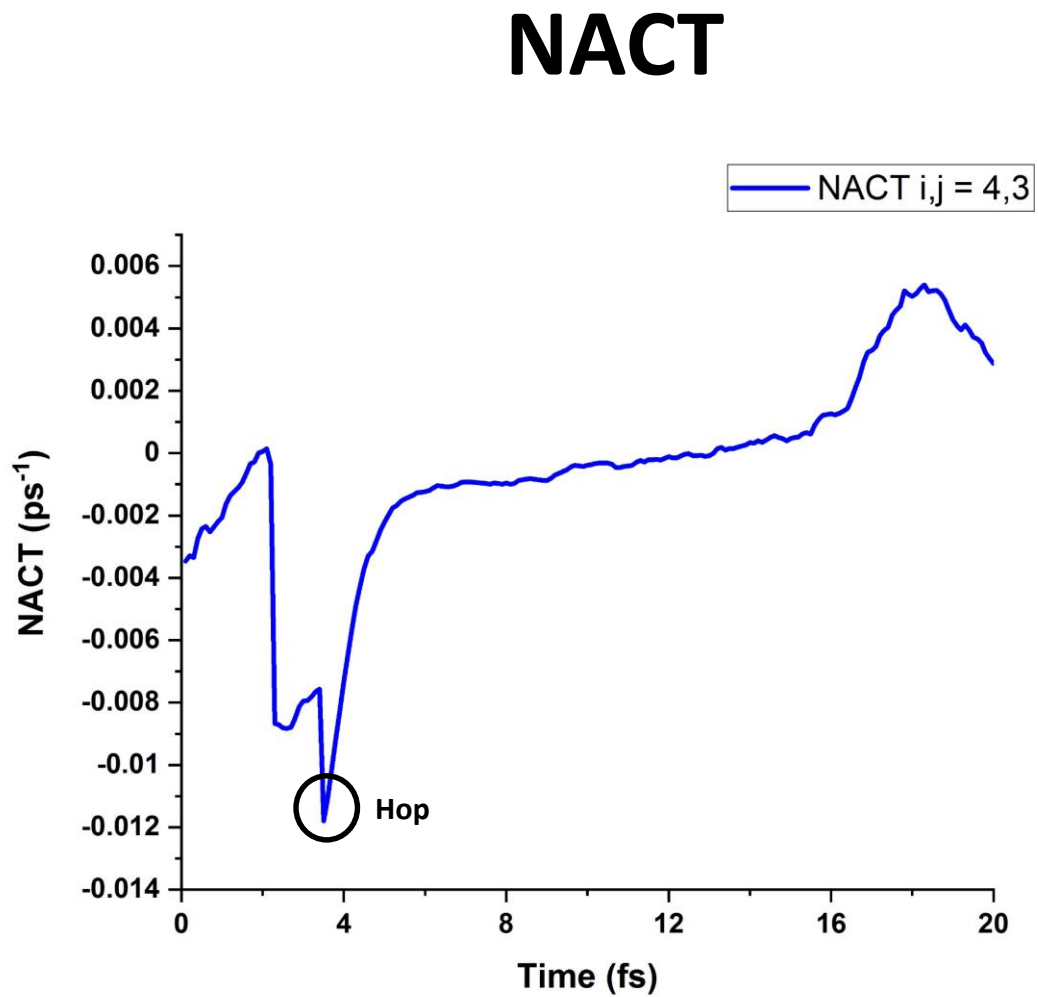
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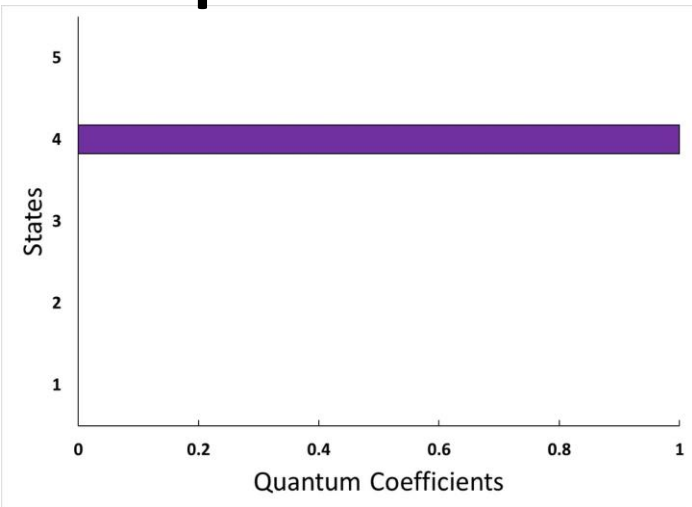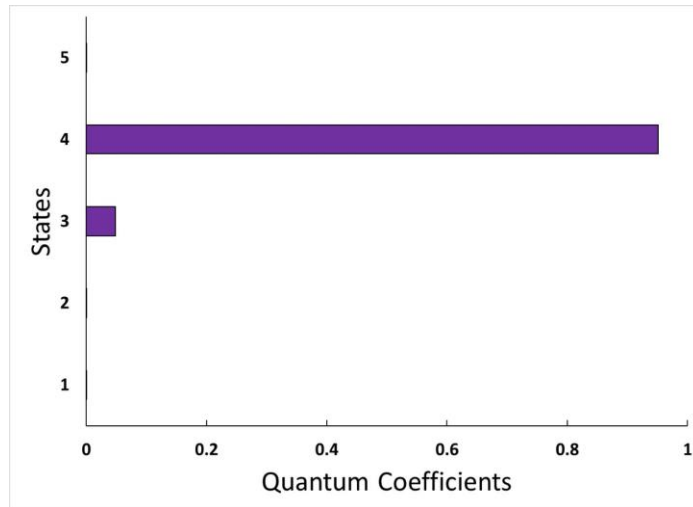- Bonus Development Features

**Benzene: PES**
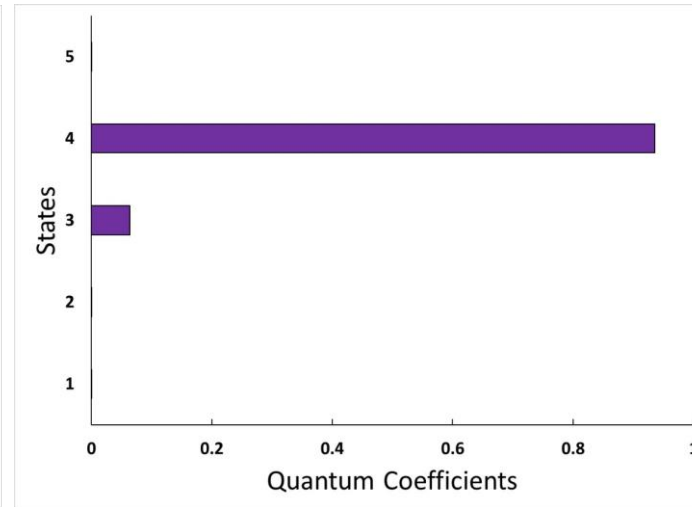
**NACT**
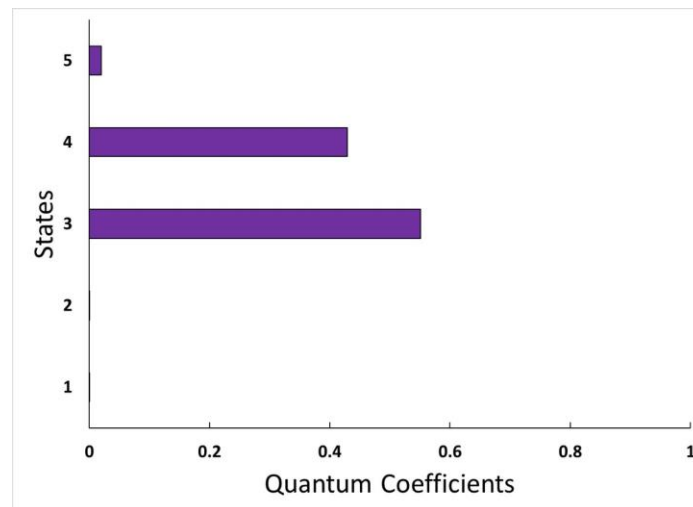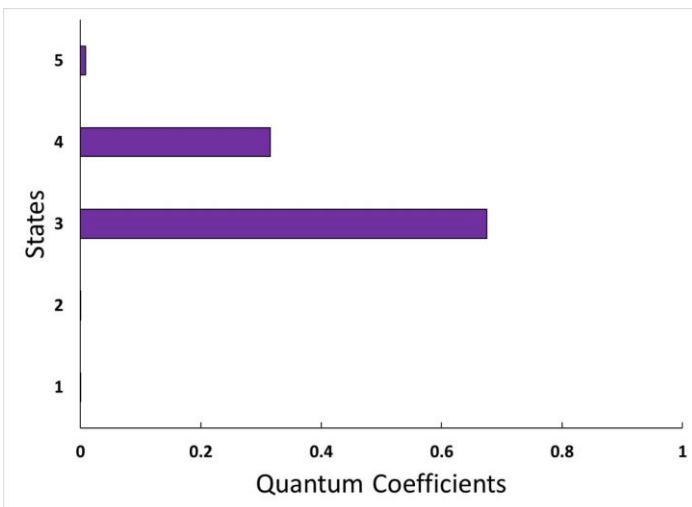
**PES**

# Quantum Coefficients
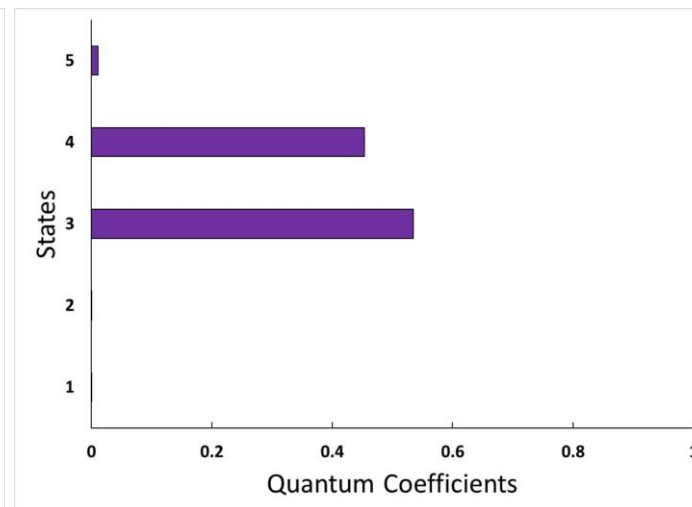
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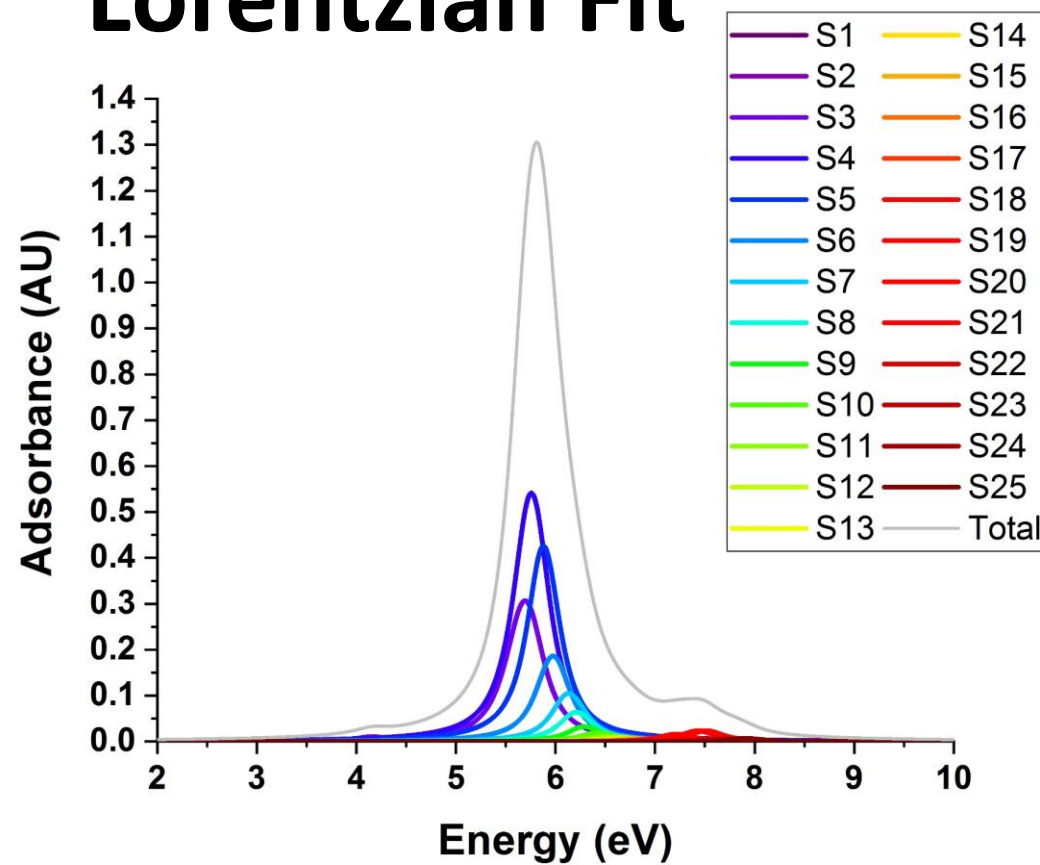  - **Analysis**
- Bonus Development Features
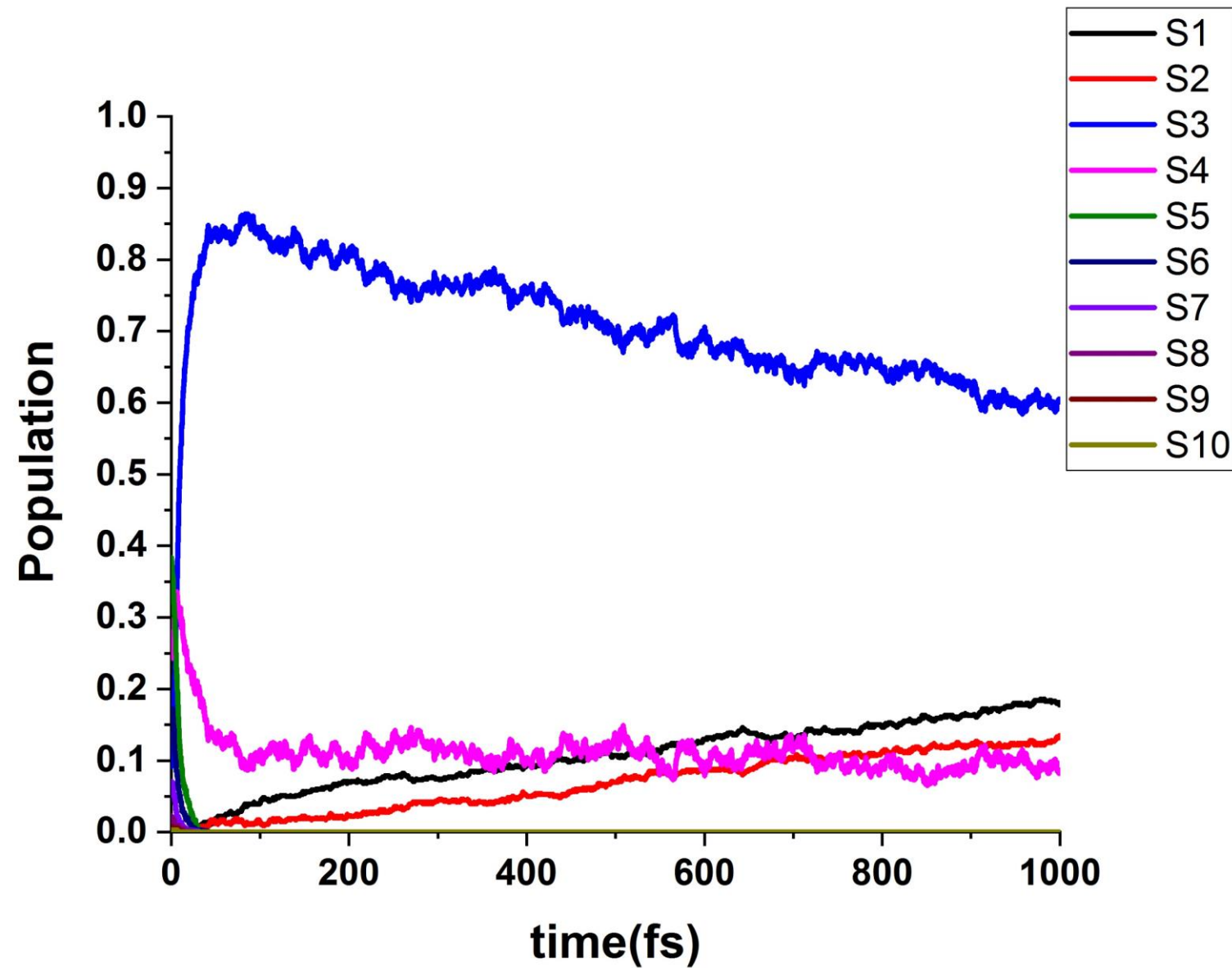
**Swarms of Trajectories**

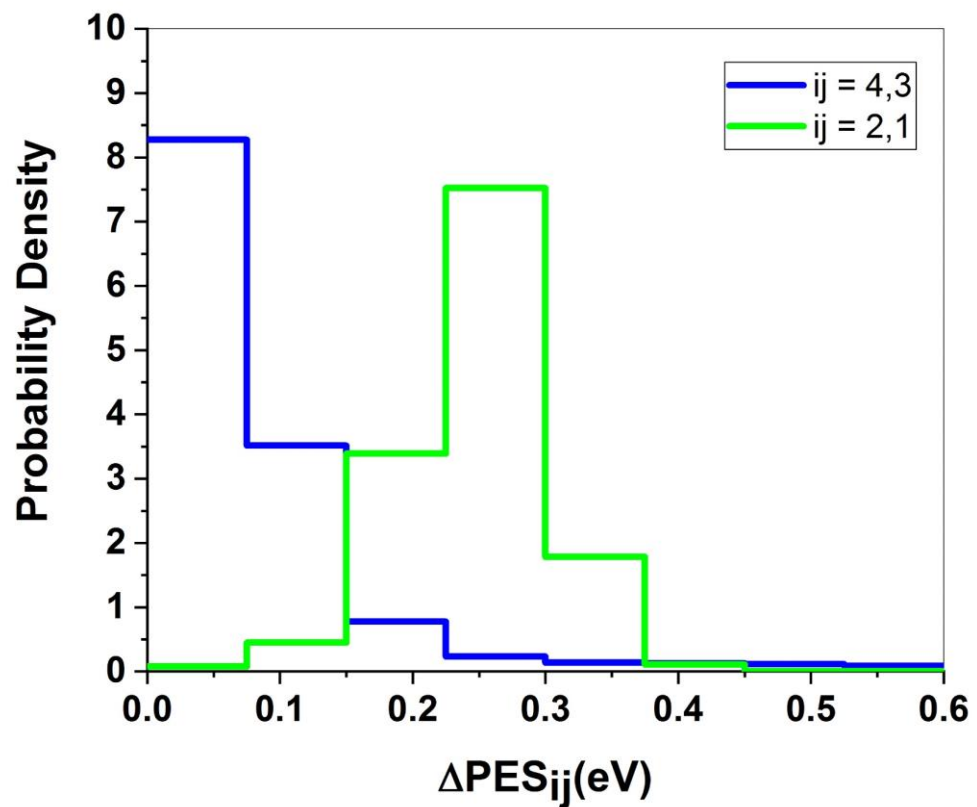# Benzene:Spectrum
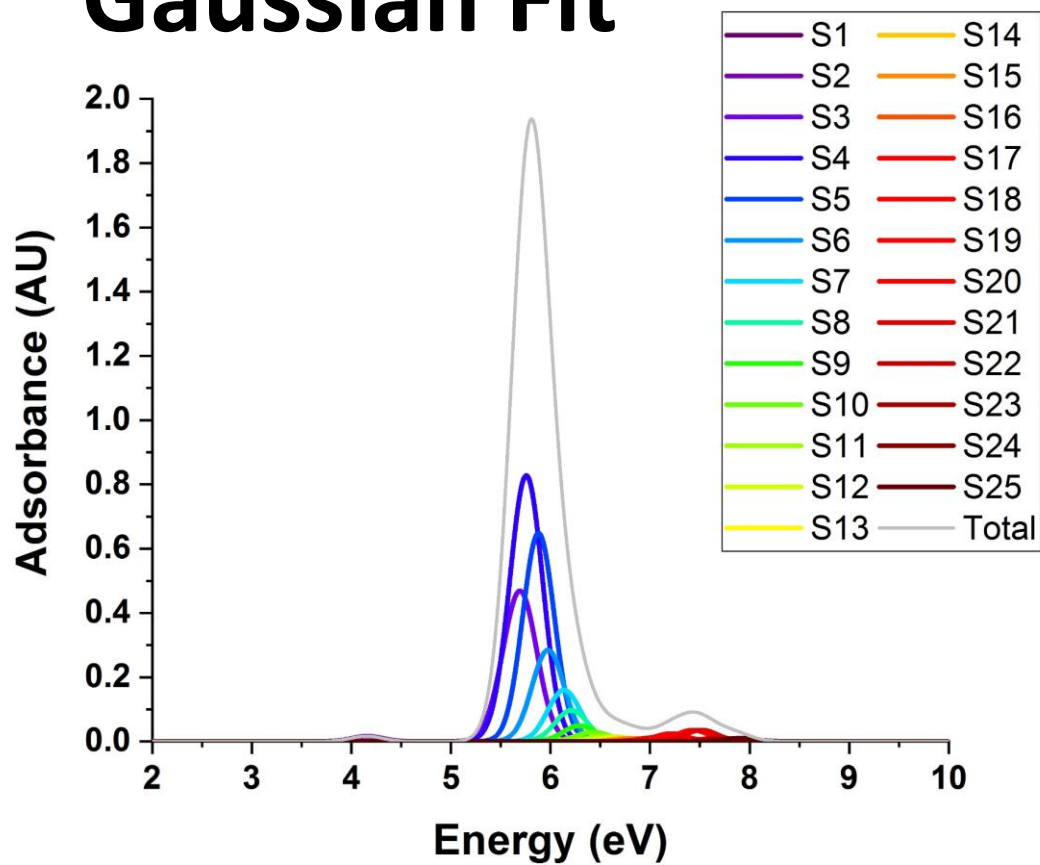
# Populations

## Benzene

# PES:Benzene

**Total**

**At Hop**
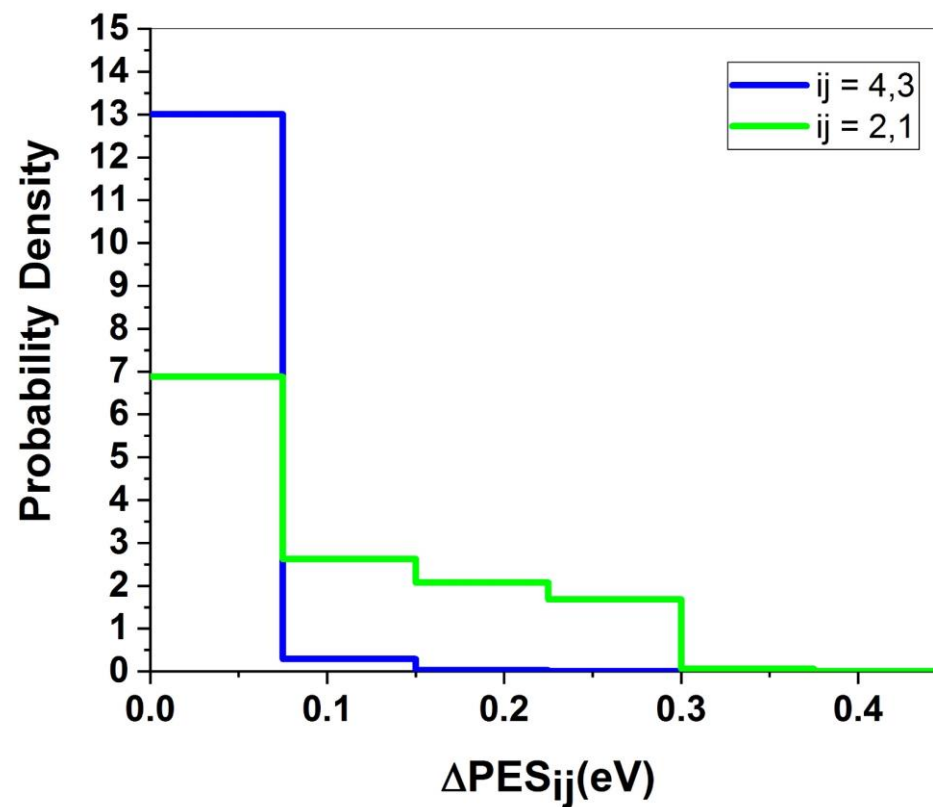
**Benzene**
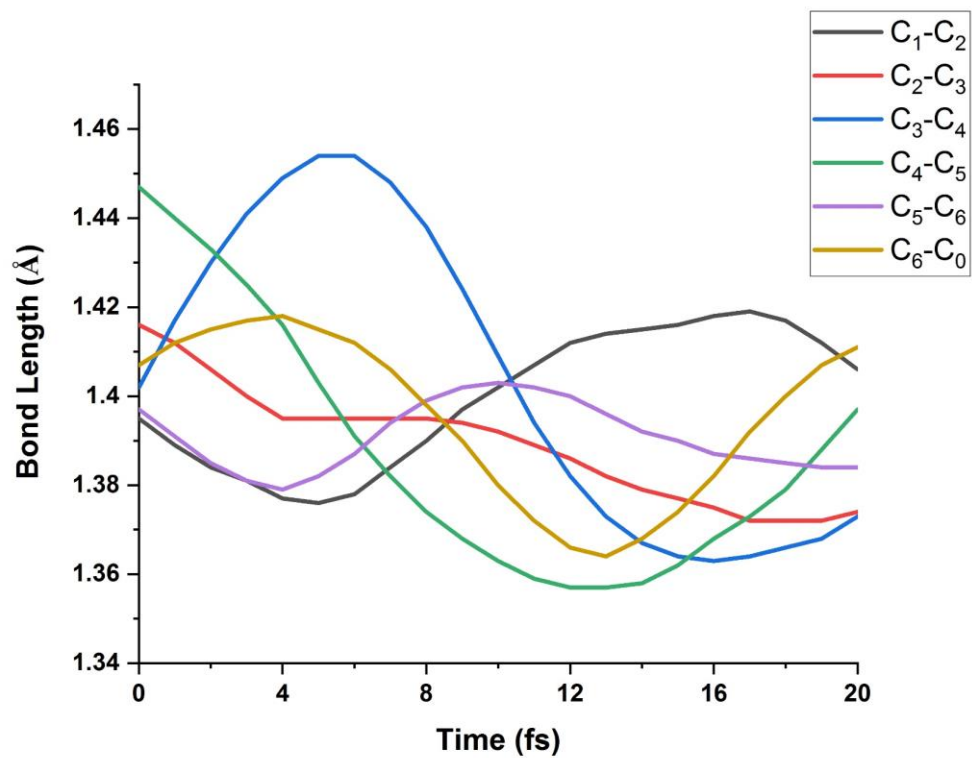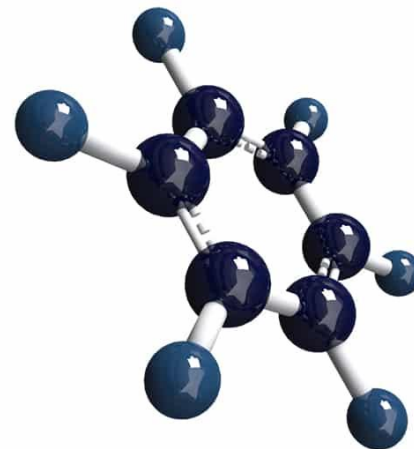
**GST**

**Ensemble**

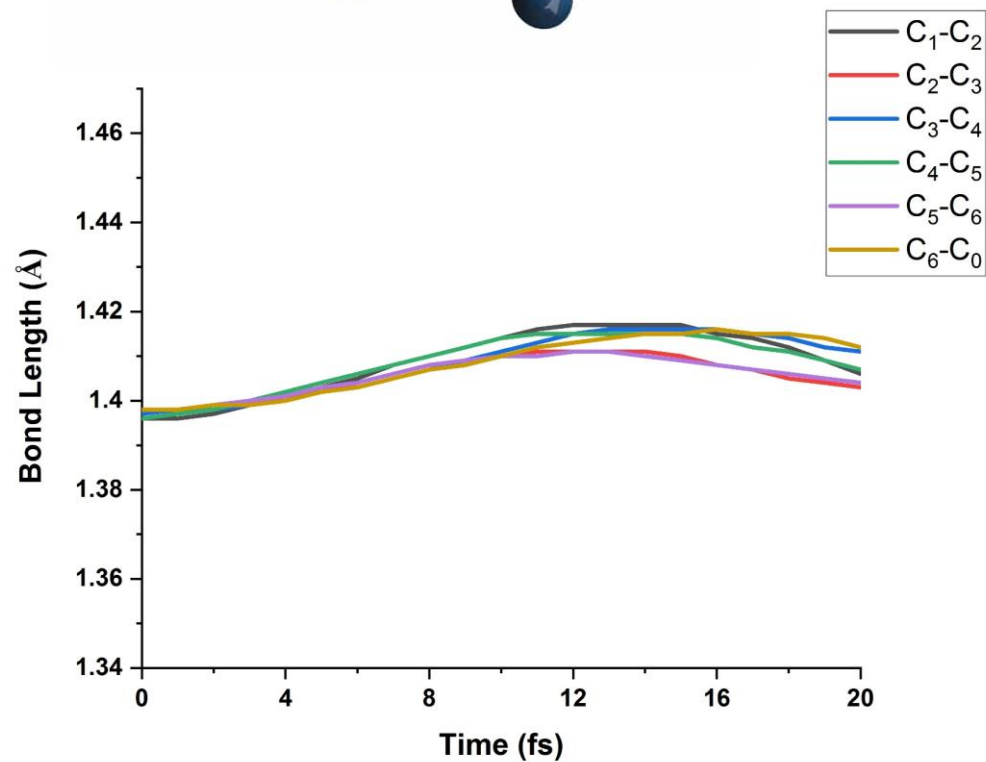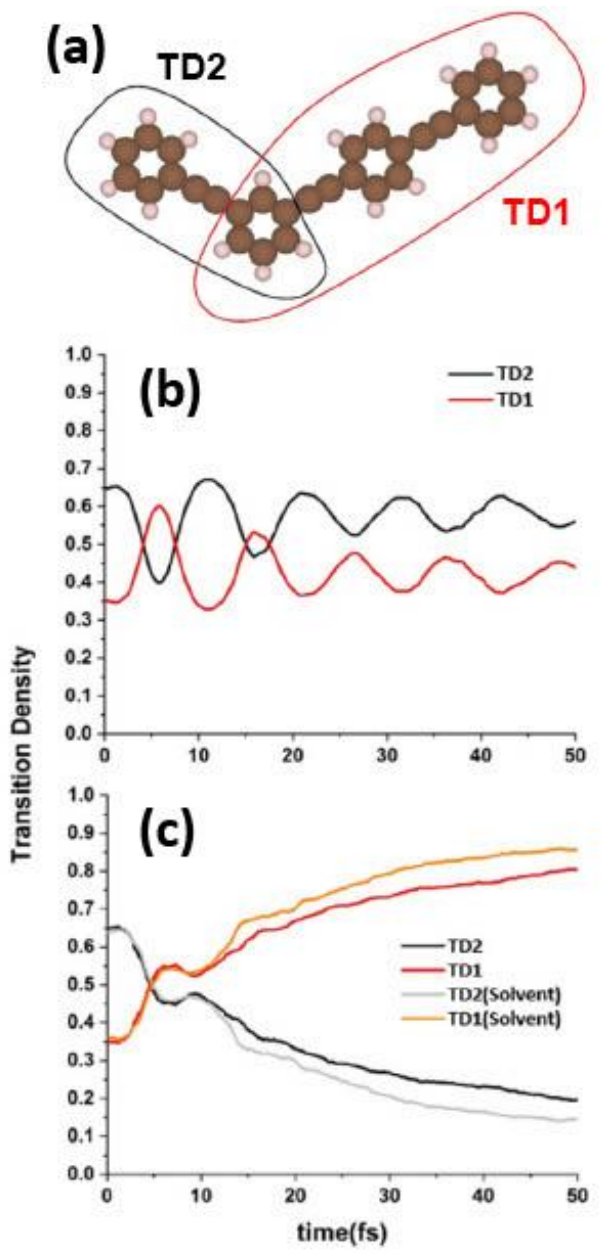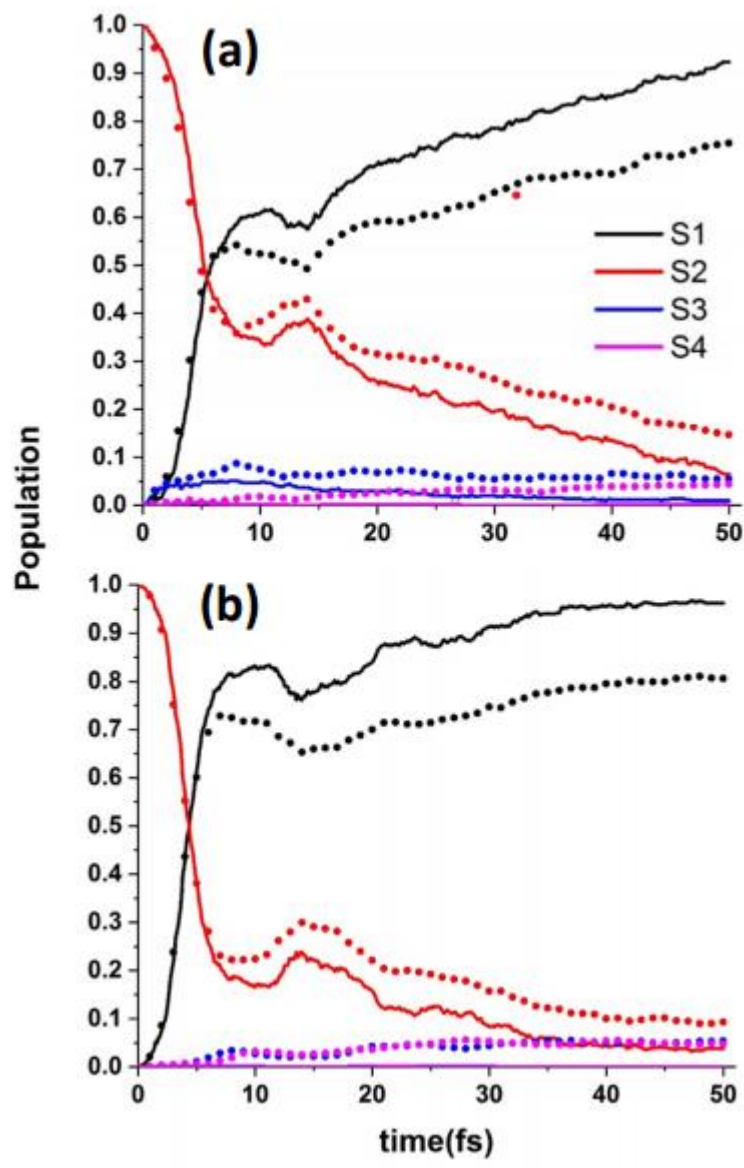**polyphenylene ethynylene dendrimer: Populations and Transition Densities**

# Nitromethane