Hang on...

What was this story about decoherence?

Credit: J. Michl and V. Bonacic-Koutecký, "Electronic Aspects of Organic Photochemistry". John Wiley and Sons, Inc., New York, 1990.
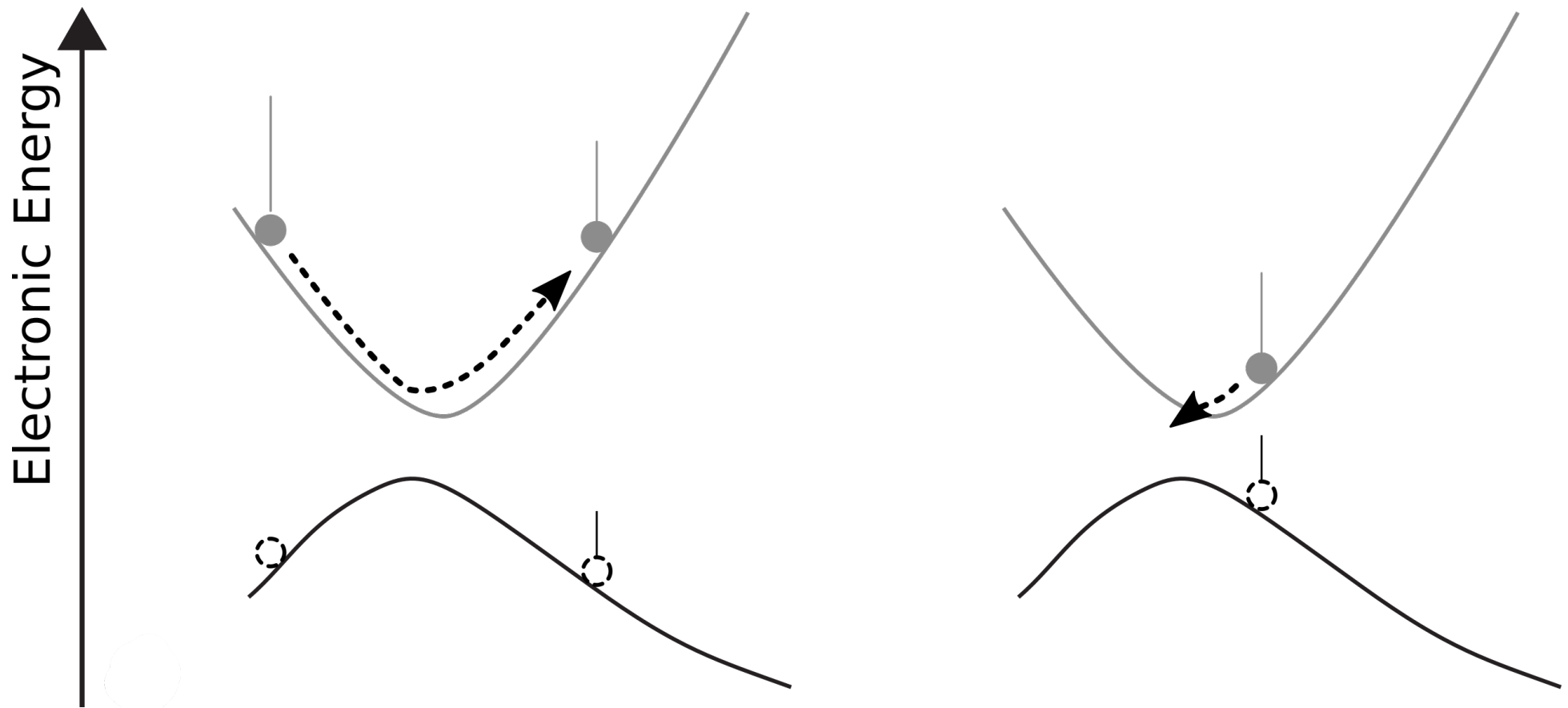
Decoherence issue in TSH

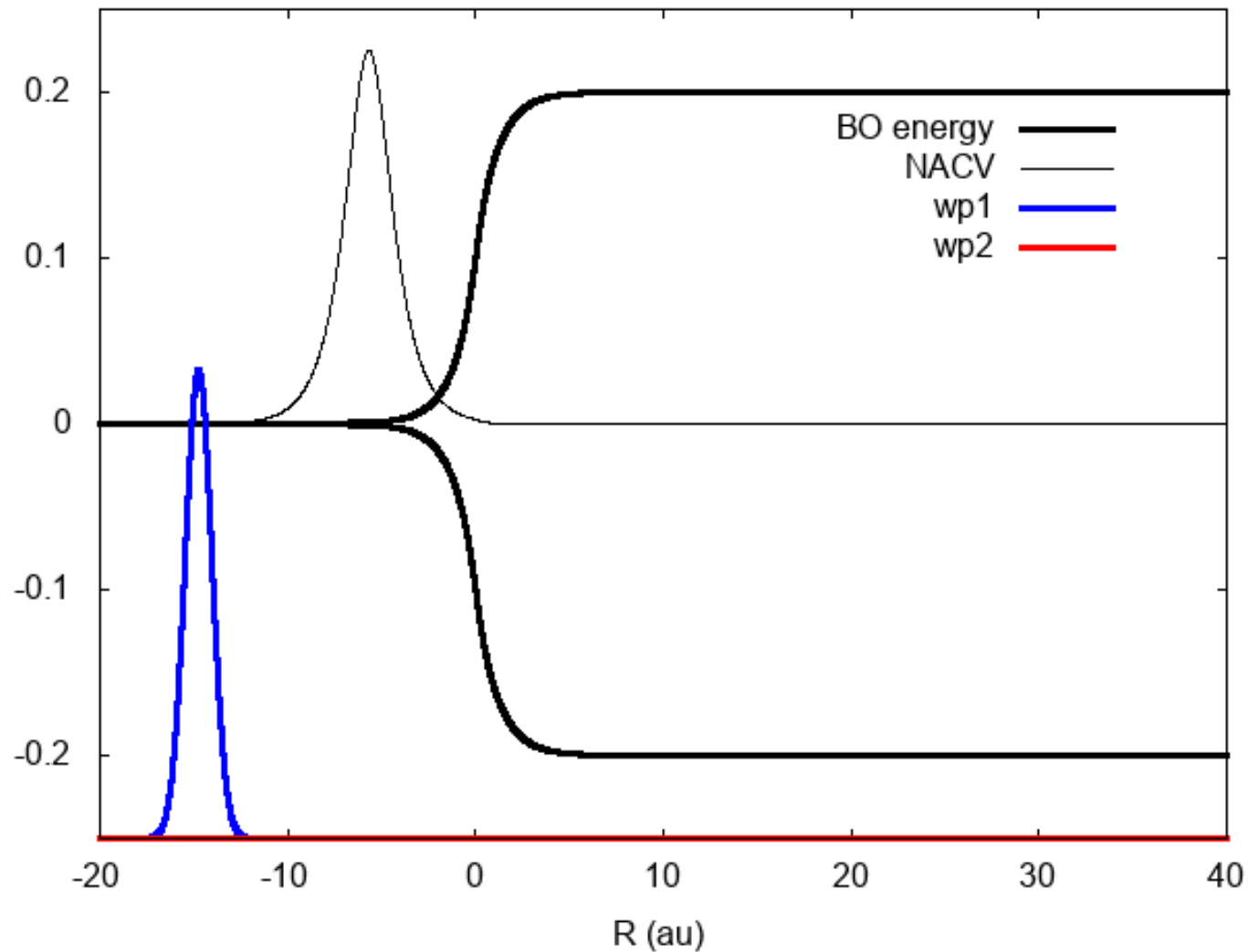**Decoherence of nuclear wavepackets in Quantum Dynamics**
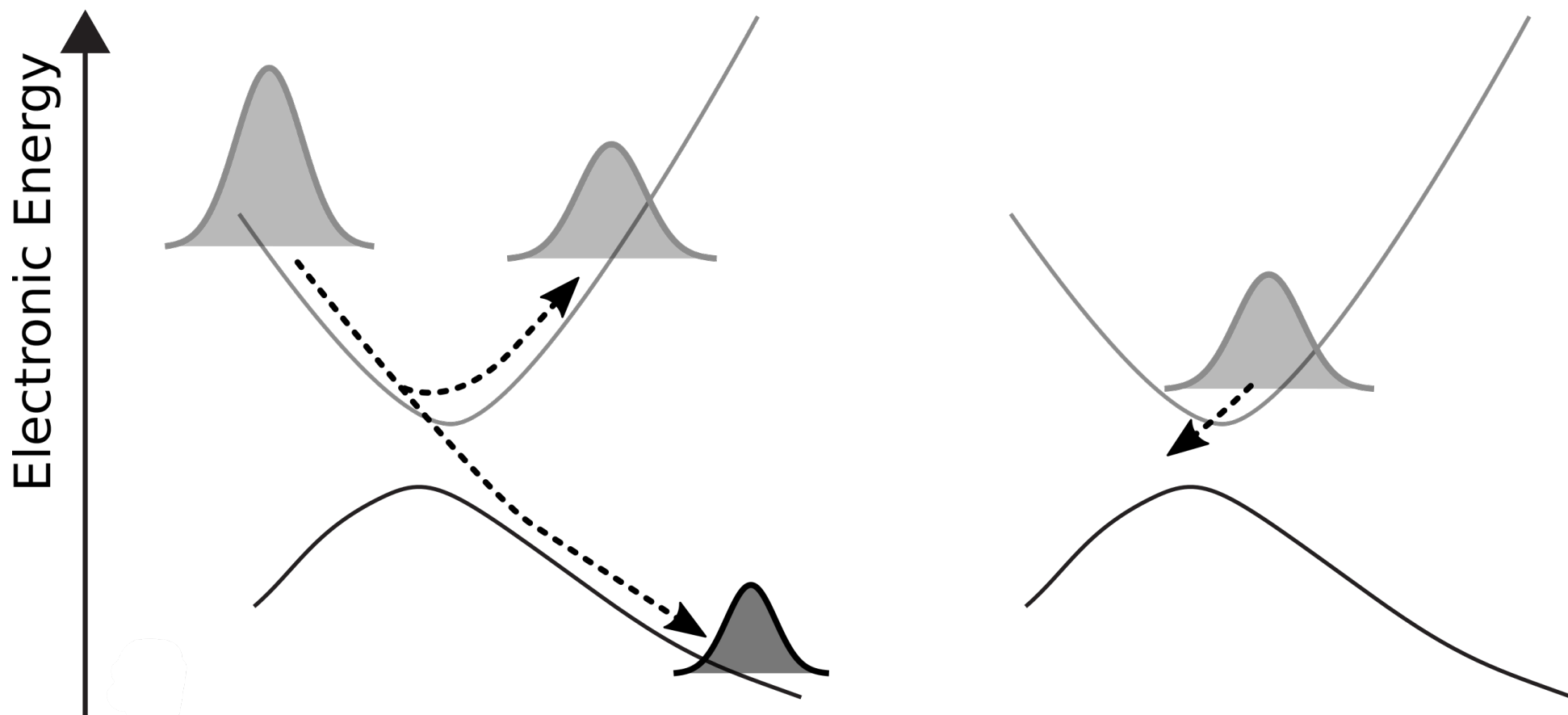
Decoherence issue in TSH

'Overcoherence' of nuclear wavepackets in Trajectory Surface Hopping

TSH and decoherence – example with a model system
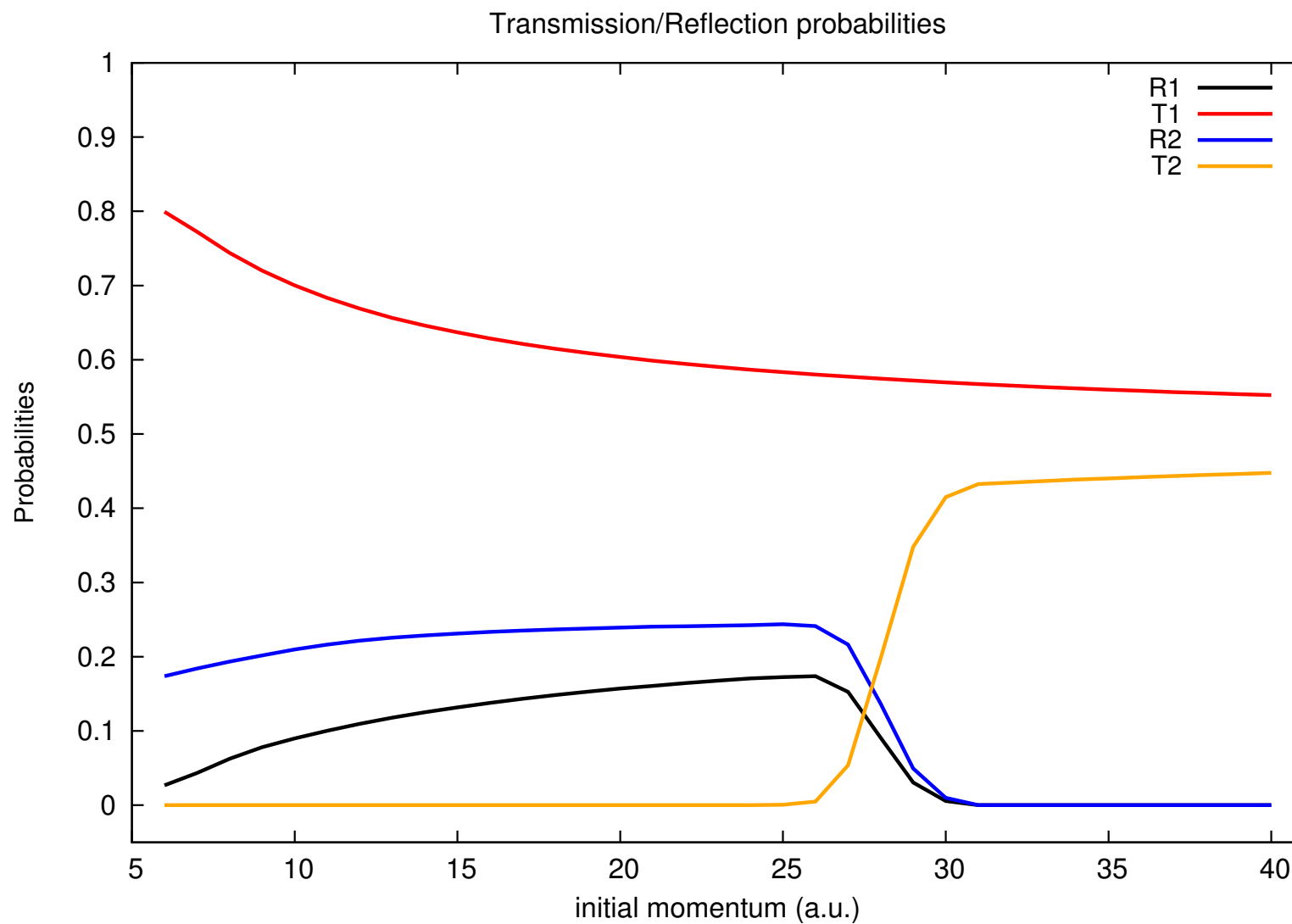
Tully model 3 – a challenge for decoherence. **Quantum Dynamics**
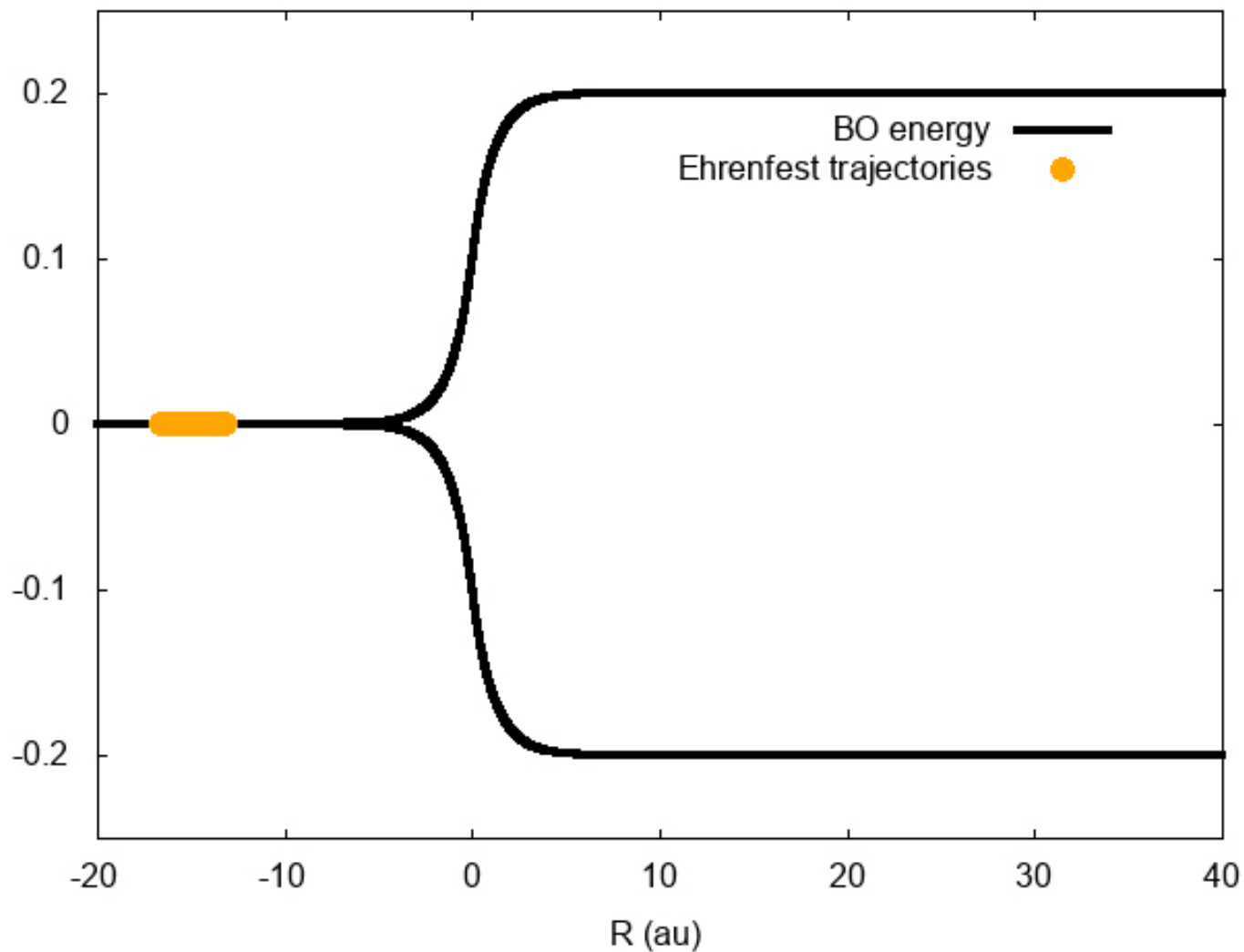

Credit movie: Federica Agostini

TSH and decoherence – example with a model system

Exact quantum dynamics

Transmission/Reflection probabilities

TSH and decoherence – example with a model system
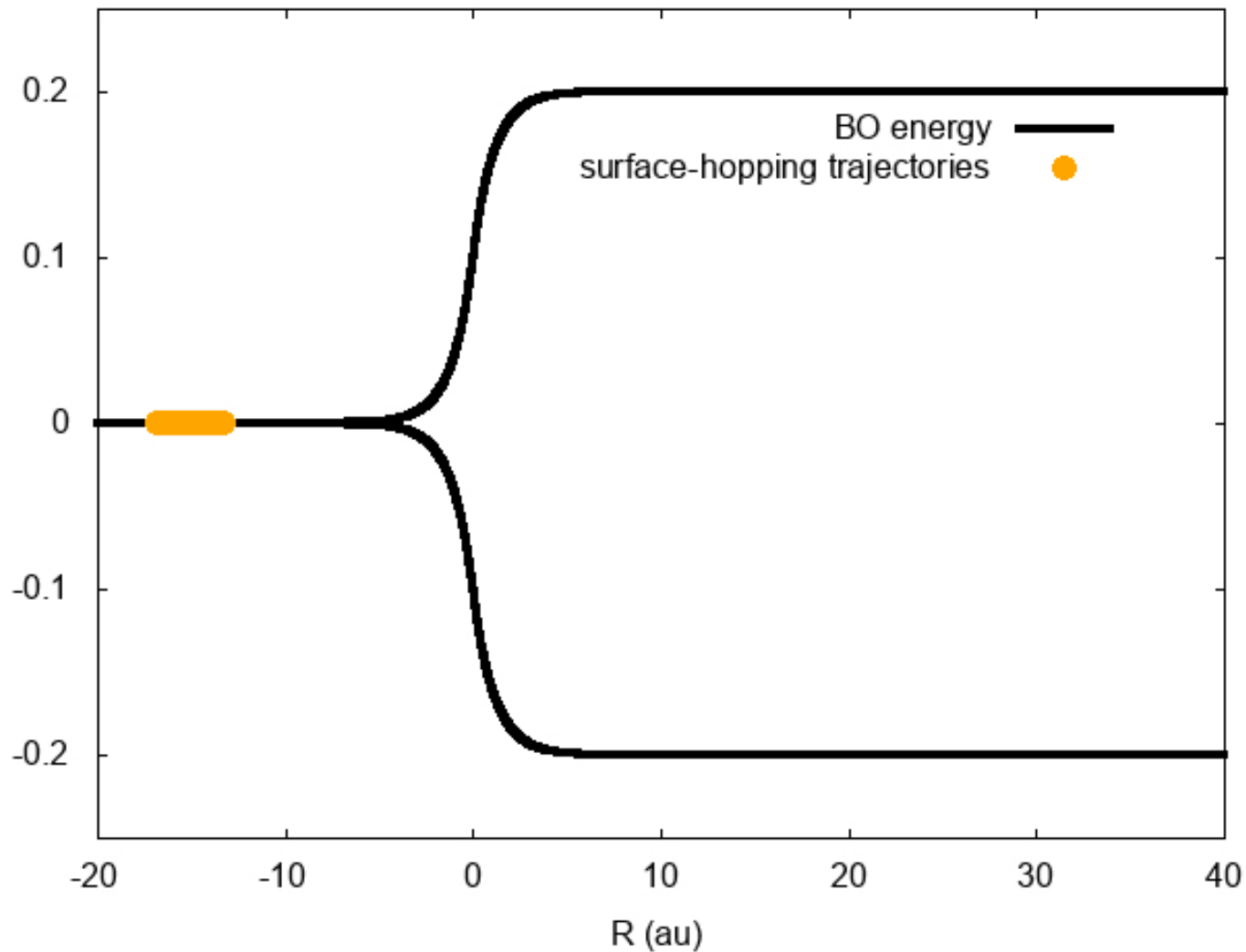
Tully model 3 – a challenge for decoherence. **Ehrenfest dynamics**

Credit movie: Federica Agostini

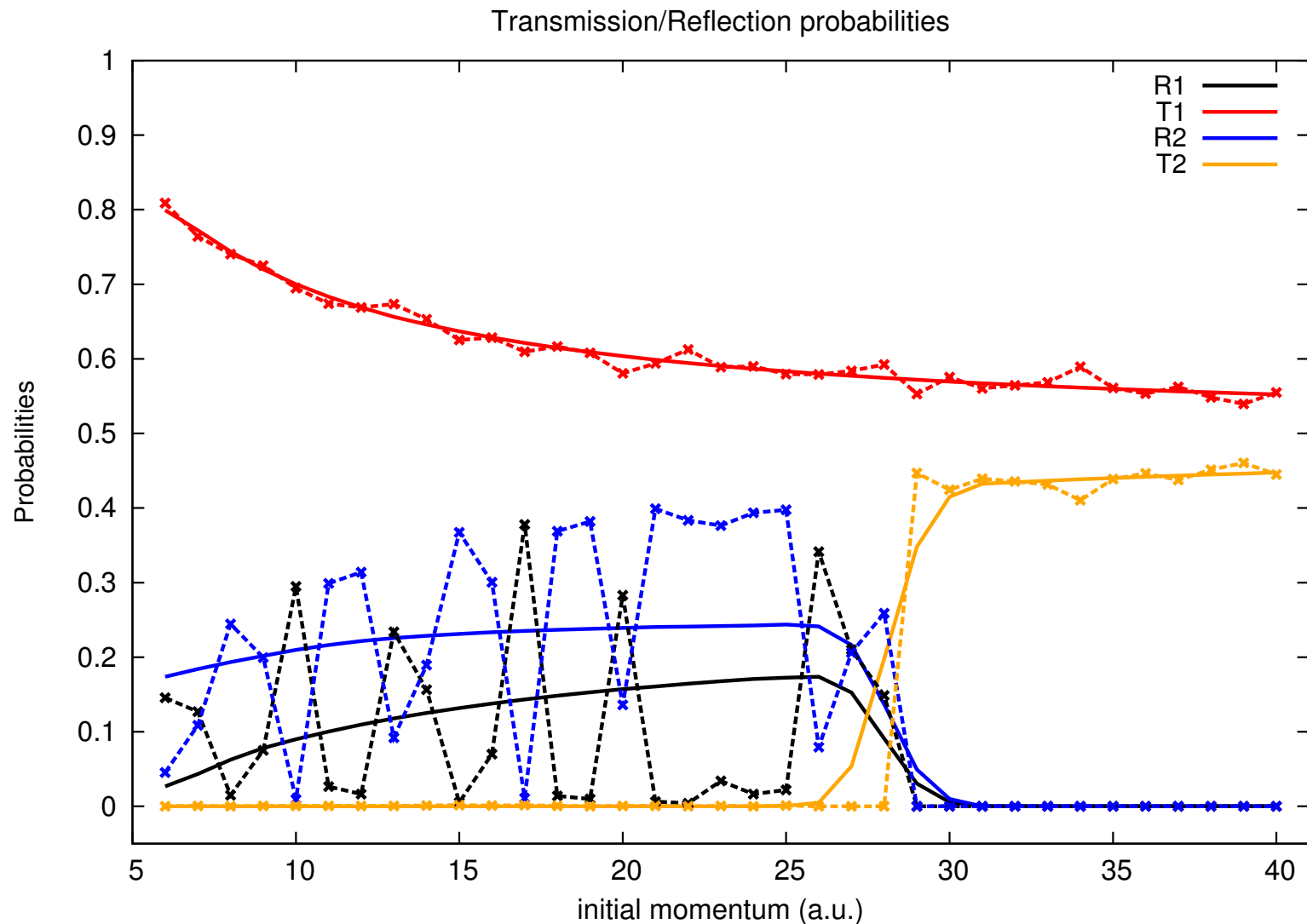# TSH and decoherence – example with a model system

Tully model 3 – a challenge for decoherence. TSH
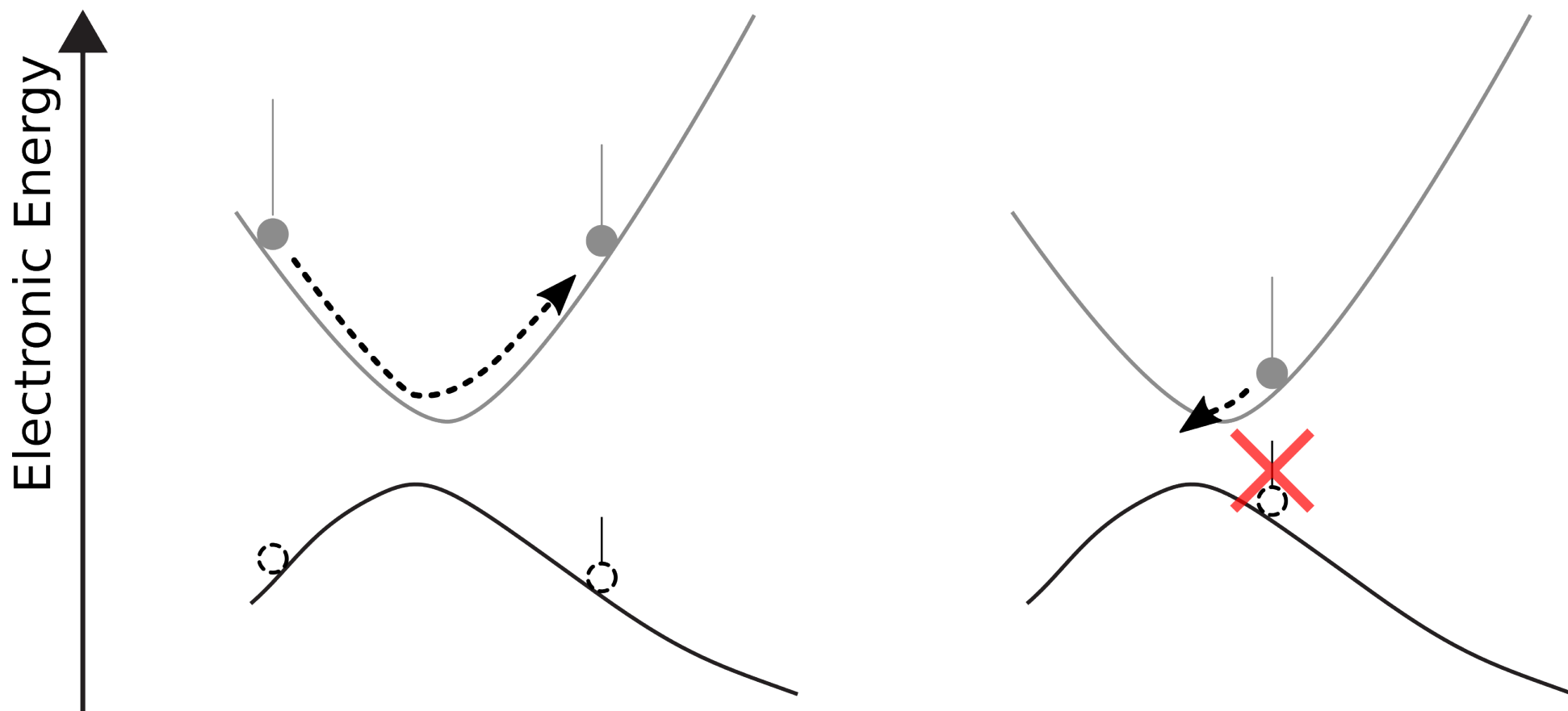

Credit movie: Federica Agostini

TSH and decoherence – example with a model system

TSH, in its original form, struggle to describe decoherence effects.

Transmission/Reflection probabilities

Decoherence issue in TSH

Ad hoc decoherence correction for Trajectory Surface Hopping

Decoherence corrections have been developed – energy-based decoherence correction (EDC) or augmented fewest-switches.
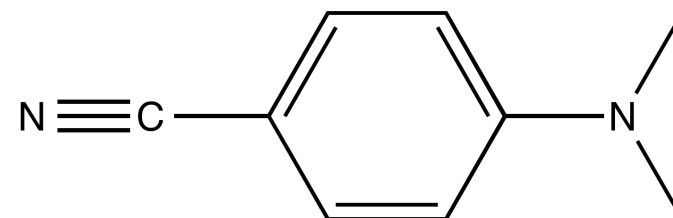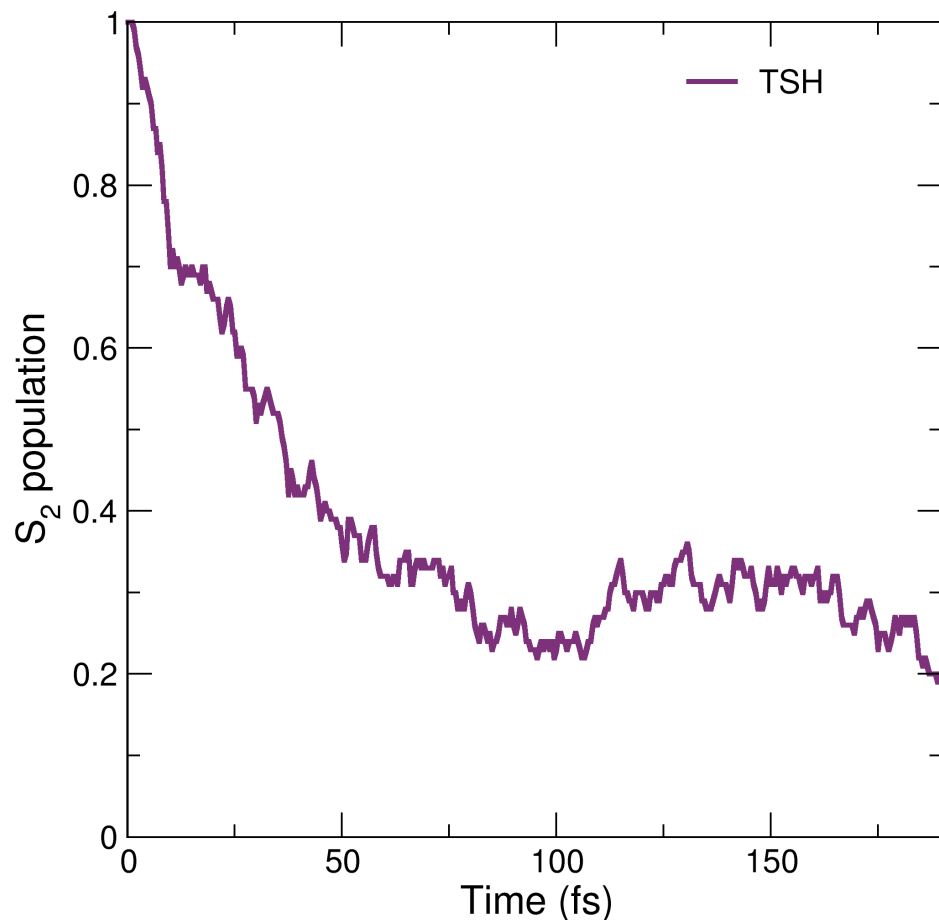See G. Granucci and M. Persico, *J. Chem. Phys.*, **126**, 134114 (2007).

TSH and decoherence – molecular example

Is TSH overcoherence a problem at all for molecular applications?

TSH and decoherence – molecular example

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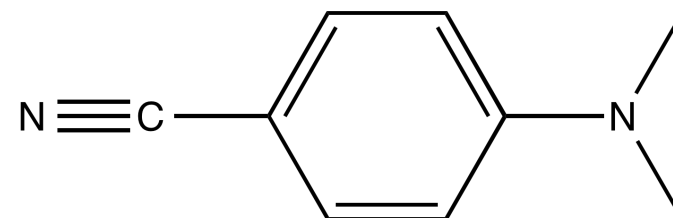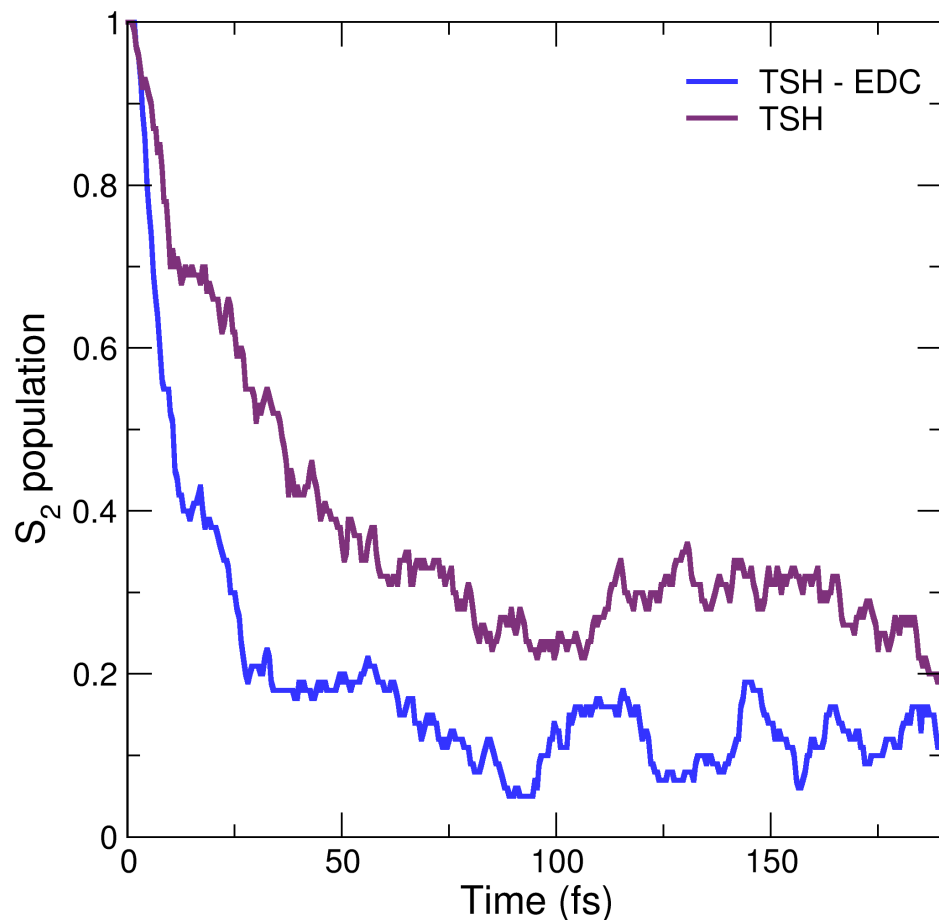

Nonadiabatic decay of the molecule DMABN following photoexcitation in its S_2 electronic state.

TSH with no decoherence correction, 100 independent trajectories, LR-TDDFT/TDA.

TSH and decoherence – molecular example

Is TSH overcoherence a problem at all for molecular applications?
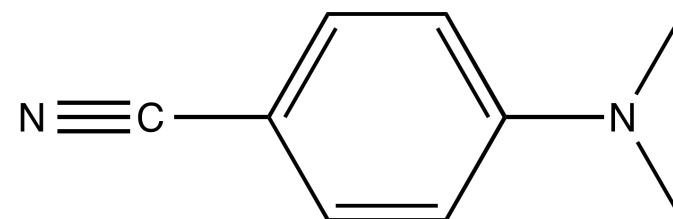

Nonadiabatic decay of the molecule DMABN following photoexcitation in its S_2 electronic state.

TSH without and with (EDC) decoherence correction, 100 independent trajectories, LR-TDDFT/TDA.

TSH and decoherence – molecular example

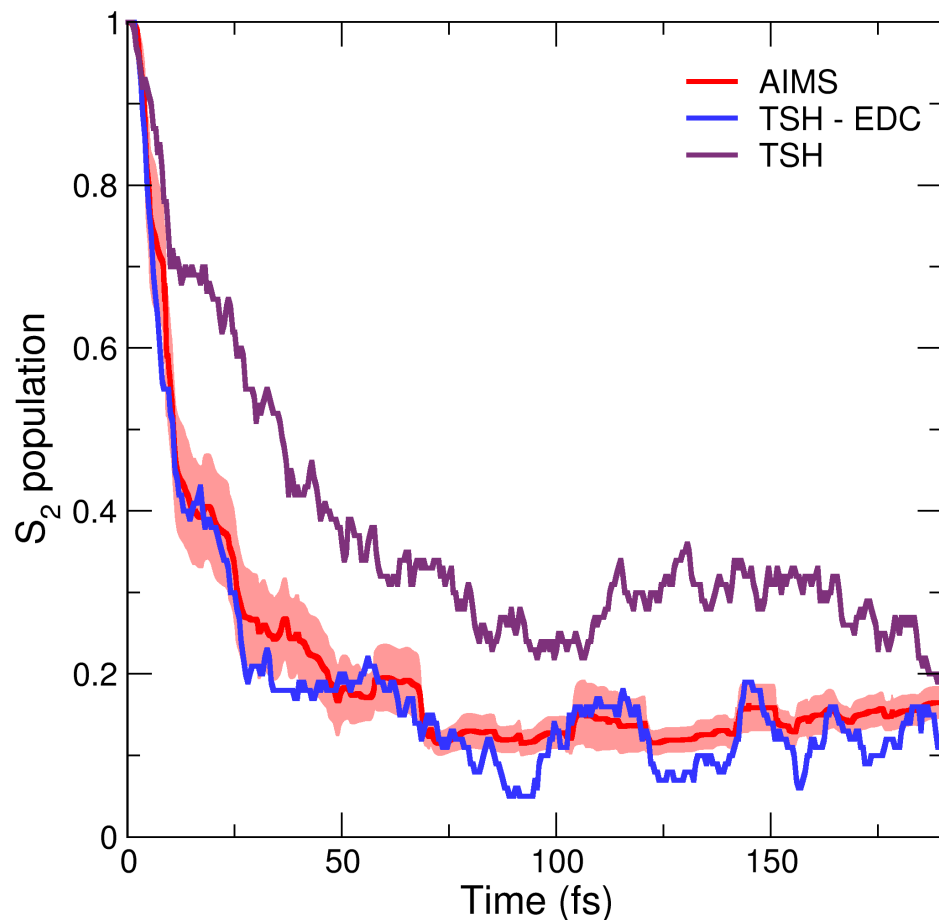**Is TSH overcoherence a problem at all for molecular applications?**

Nonadiabatic decay of the molecule DMABN following photoexcitation in its S_2 electronic state.

TSH without and with (EDC) decoherence correction, 100 independent trajectories, LR-TDDFT/TDA.

AIMS, 24 parent TBFs, LR-TDDFT/TDA.

Decoherence issue in TSH

Decoherence of nuclear wavepackets in Ab Initio Multiple Spawning