CFEL SCIENCE

SEMINAR

28th October 2020 - 2:00 p.m.

Virtual meeting room in ZOOM (ID: 975 5069 7074 / PW: 642214)

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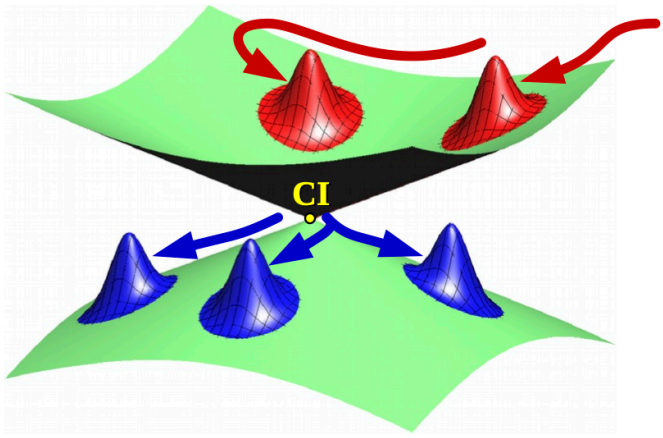
Quantum non-adiabatic dynamics with Gaussian wavepackets

Quantum methods scale exponentially with the number of particles. It prevents full quantum simulations of large molecular systems. Employing time-dependent Gaussian basis functions helps fighting this limitation by allowing “on-the-fly” evaluation of the potential energy surfaces (PESs) at a lower number of nuclear geometries compared to methods using large dimensional grids. We will focus on non-adiabatic processes when nuclei are strongly coupled to electrons and quantum simulations are necessary.

I will touch on some recently introduced improvements related to the choice of the electron-nuclear basis and open systems: 1) to deal with singular Hamiltonian terms that appear when PESs intersect, 2) to generalize spawning or cloning procedures to ensure convergence in full quantum simulations, and 3) to treat open systems with Gaussian basis functions using a Schrödinger equation approach.



Gaussian wavepacket evolving at a conical intersection

References:

1) L. Joubert-Doriol and A. F. Izmaylov: *J. Chem. Phys.* **148**, 114102 (2018).

2) A. F. Izmaylov and L. Joubert-Doriol: *J. Phys. Chem. Lett.* **8**, 1793 (2017).

3) L. Joubert-Doriol and A. F. Izmaylov: *J. Chem. Phys.* **142**, 134107 (2015).

Host: Robin Santra – CFEL-DESY Theory Division