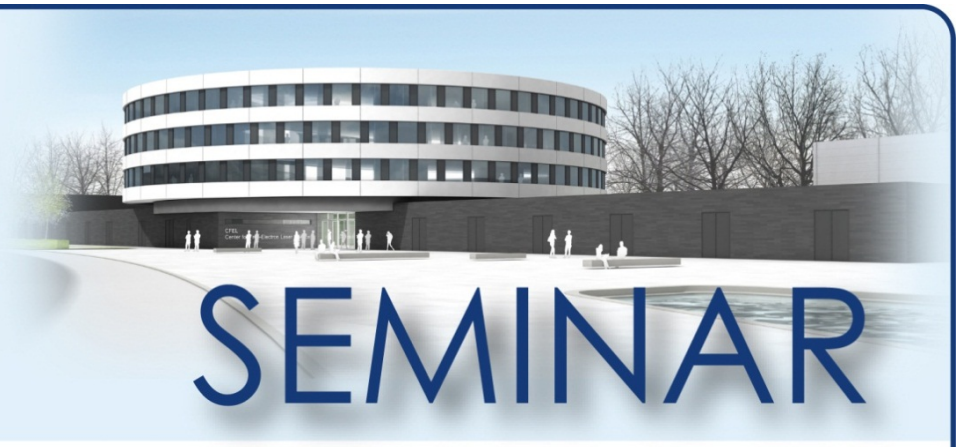
CFEL SCIENCE



SEMINAR

3rd June 2020 - 2:00 p.m.

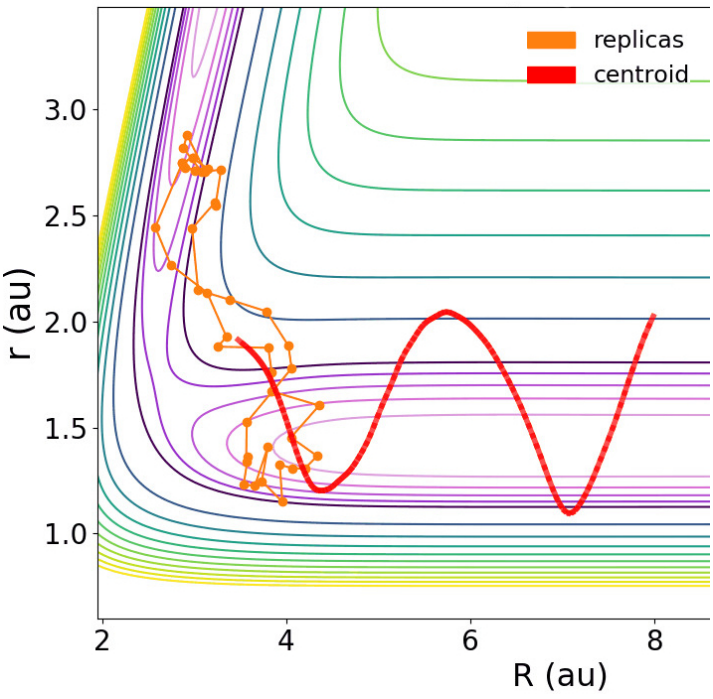
Virtual meeting room in ZOOM (ID: 940 7601 8812 / PW: 294783664)

Adrien Marjollet

Center for Free-Electron Laser Science, DESY, Germany

Extracting approximate state-resolved cross sections from ring polymer molecular dynamics

Detailed knowledge of gas-phase reactions for specific initial states of the reaction partners is important to understand the dynamics and the role of the different forms of energy involved (e.g. translational, vibrational, and rotational). However, detailed studies of reaction dynamics through rigorous quantum dynamical simulations are computationally infeasible for most polyatomic reactions. We will present an approach to obtain approximate quantum state-selective reactive cross sections that approximately includes quantum effects like zero-point energy and tunneling. It does so with computational efficiency by employing an extension of the ring polymer molecular dynamics approach. We will then show and discuss the first encouraging results of our approach applied to the prototypical X + H_2(v=0,1) reactions, where X = Mu, H, D, F, and Cl.



Ring polymer in reaction coordinates stretching over the reaction barrier

[1] A. Marjollet and R. Welsh, *J. Chem. Phys.* **152**, 194113 (2020).

Host: Robin Santra – CFEL-DESY Theory Division