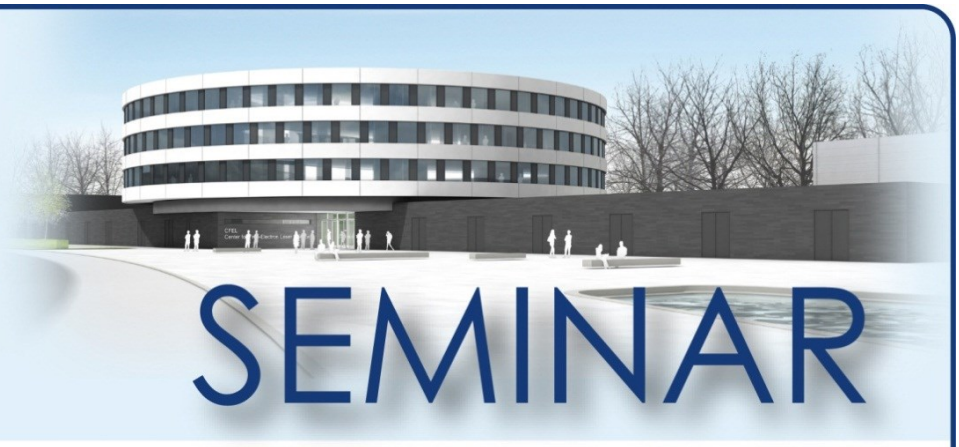
CFEL SCIENCE



SEMINAR

22nd November 2017 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

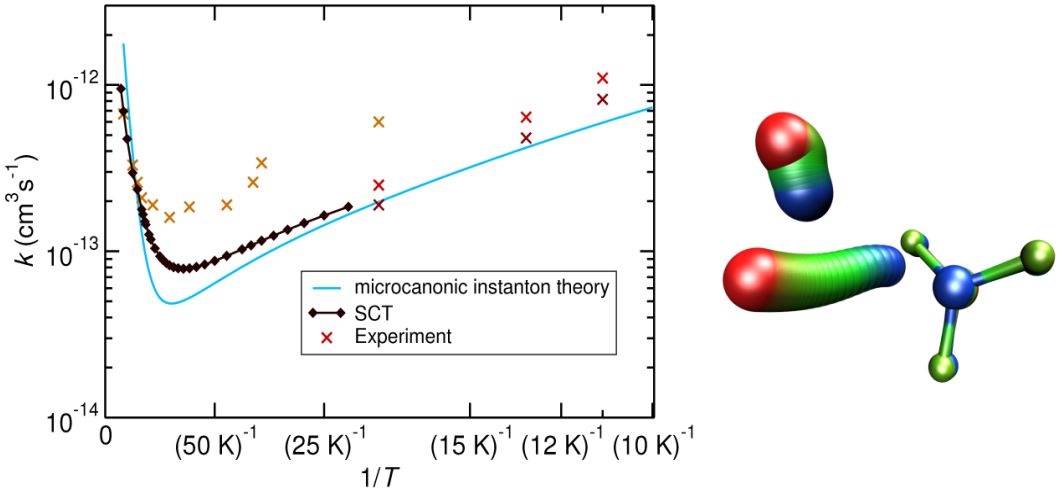
Johannes Kästner

Institute for Theoretical Chemistry, University of Stuttgart, Germany

Improvements of instanton theory to simulate atom tunneling in astrochemical reactions

Instanton theory, based on Feynman path integrals, is increasingly used for accurate prediction of reaction rate constants. We present methodological improvements in several aspects: its accuracy close to the crossover temperature and its limit below that temperature, its convergence properties with the number of images, its temperature-dependence for bimolecular rate constants at low temperature, as well as its dependence on the quality of the potential. Some of these aspects were improved on by using a microcanonical formulation of instanton theory.

We applied instanton theory to several reactions of astrochemical interest. Atom tunneling allows reactions to proceed at the cryogenic temperatures of the interstellar medium despite a reaction barrier. These help to explain the formation of water and of the first building blocks of life.



Rate constants and instanton path for the reaction $NH_3^+ + H_2 \rightarrow NH_4^+ + H$ [5].

Host: Robin Santra – CFEL-DESY Theory Division