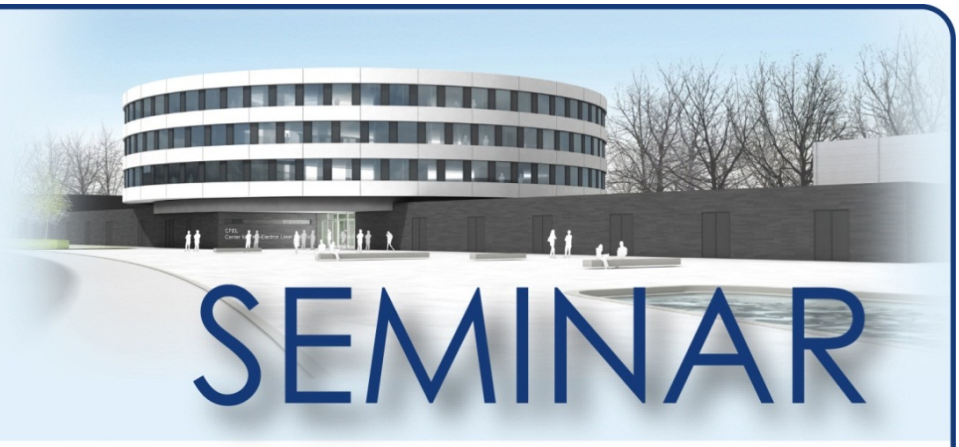
CFEL SCIENCE



SEMINAR

31st January 2024 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

Jonathan Mannouch

Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

A mapping approach to surface hopping

Processes involving beyond Born-Oppenheimer dynamics are common in chemistry, including photoinduced ultrafast relaxation through conical intersections and electron-transfer reactions in solution. Fewest-switches surface hopping (FSSH) [1] is currently the most popular approach for simulating such processes. However, FSSH lacks a complete formal derivation from first principles and is known to suffer from the so-called 'overcoherence error' that requires ad hoc decoherence corrections to fix.

In this talk, I will introduce a recently derived semiclassical trajectory approach called the mapping approach to surface hopping (MASH) [2]. Through its application to a selection of molecular systems, I will demonstrate that MASH provides accurate surface-hopping dynamics without the need for decoherence corrections, exhibiting improved accuracy over FSSH at a comparable computational cost.

[1] J. E. Subotnik *et al.*, *Annu. Rev. Phys. Chem.* **67**, 387–417 (2016).

[2] J. R. Mannouch & J. O. Richardson, *J. Chem. Phys.* **158**, 104111 (2023).

Host: Robin Santra – CFEL-DESY Theory Division