

The director general of HUN-REN Wigner Research Centre for Physics
invites applications for a postdoctoral position

We have an opening for a 2-year full-time postdoc position in computational ultrafast excited-state dynamics in the Femtosecond Spectroscopy and X-ray Spectroscopy group at HUN-REN Wigner Research Centre for Physics (Budapest, Hungary). The research is an integral part of the project „Simulation of Ultrafast Dynamics in Photofunctional Transition Metal Complexes” led by Mátyás Pápai.

In this project, we investigate excited-state mechanisms of photofunctional transition metal complexes (such as photoswitchable Fe(II) complexes and light harvesters) by simulation of ultrafast excited-state dynamics. The utilized computational techniques include trajectory surface hopping (TSH) and machine learning (ML), which we will use to calculate potential energy surfaces for spin-vibronic dynamics; importantly, this will push boundaries of excited-state dynamics simulations both in terms of molecular size and timescales. Combining our simulations with the ultrafast experiments carried out by the group (optical and X-ray spectroscopy at our in-house labs and large-scale facilities), we are making efforts to resolve complex ultrafast dynamics in photofunctional transition metal complexes.

Relevant recent publications

<https://doi.org/10.1039/D3TA05985E>
<https://doi.org/10.1038/s42004-022-00796-z>

Qualifications

- PhD in theoretical chemistry or molecular physics
- Experience in quantum chemistry and molecular dynamics
- Coding skills in Python/Fortran
- English language (written and oral)

The ideal candidate would also possess experience in ML and its application in quantum chemistry and/or molecular dynamics.

Tasks

- Carrying out and analyzing TSH simulations
- Implementation of the ML module for spin-vibronic dynamics
- Calculation of time-dependent experimental observables (optical and X-ray spectroscopy)

Research group

The theory team of the Femtosecond Spectroscopy and X-ray Spectroscopy research group currently consists of two senior researchers and a postdoc. The group operates in-house X-ray spectroscopy and transient optical absorption spectroscopy (TOAS) instruments and regularly perform time-resolved experiments at synchrotrons and X-ray free electron lasers (XFELs). For a summary of recent scientific achievements of the group, see:

<https://wigner.hu/nuklearis-anyagtudomanyi-osztaly/mta-lendulet-femoszekundumos-spektroszkopia-es/research>

Salary and allowances: As agreed upon.

Application process

The position is available from 1st January 2025, note, however that the start date can be made flexible, starting earlier (if agreed in time). Applications should be sent to allas@wigner.hun-ren.hu; all applicants should submit a concise cover letter, a CV, a list of publications, and contact information of at least two referees no later than 30th September 2024. Applications will be reviewed until the position is filled.

Application deadline : 30th September 2024