

Dear colleagues, especially postdoc candidates,

If you are interested in

- theoretical work computing molecular spectra with modern data scientific methods,
- work in a research center with focus on energy materials hosting a synchrotron facility,
- get connected to the Helmholtz AI network,
- join a diverse, international, and interdisciplinary group with significant research freedom
- spent 2 years of postdoc in Berlin:

We are looking for somebody like you! “We” is the “Theory of Electron Dynamics and Spectroscopy” group at the Helmholtz-Zentrum Berlin (HZB) lead by PD Dr. Annika Bande.

The project “Artificial Intelligence for X-ray Absorption Spectroscopy” is a cooperation between HEREON (Geesthacht), TUHH (Hamburg) and HZB (Berlin). We seek to use graph neural networks for predicting X-ray absorption spectra (XAS) based on the most relevant molecular configurations of graphitic nanostructures. The results of these machine learning predictions shall allow a rigorous interpretation of XAS experiments executed at BESSY II, in which characteristic parts of a spectrum can be associated 1:1 with a specific functional group. It is a follow-up project to <https://doi.org/10.1021/acs.jctc.2c00255>

Are you ready? Then apply until October 16, 2022 via the HZB job page, highlighting on your experience in electronic structure calculations as well as machine learning techniques and adding some CV, letter of reverence, and records of your studies.

For a priory inquiry, please email [annika.bande@helmholtz-berlin.de](mailto:annika.bande@helmholtz-berlin.de)

We are looking forward to getting to know you,

Annika Bande

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PD Dr. habil. Annika Bande

Theory of Electron Dynamics and Spectroscopy

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