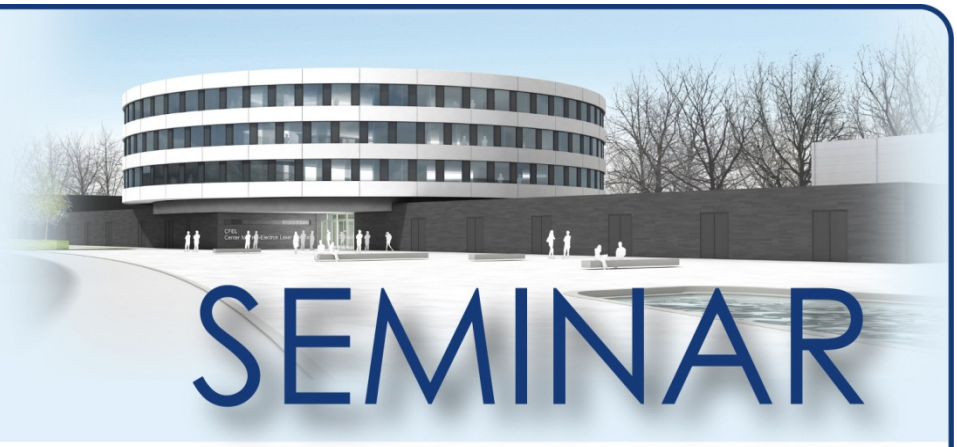
CFEL SCIENCE



SEMINAR

19 May 2022, 10:00–11:00h

CFEL - Building 99, seminar room IV (first floor)

online: https://desy.zoom.us/j/99570520017 (password: 911851)

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Deep Neural Networks for X-ray Spectroscopy: Hero or Zero?

X-ray spectroscopy delivers strong impact across the physical and biological sciences by providing end users with highly detailed information about the electronic and geometric structure of matter. To decode this information in challenging cases, e.g., in operando catalysts, batteries, and temporally evolving systems [1], advanced theoretical calculations are necessary. The complexity and resource requirements often render these out of reach for end users, and therefore, the data are often not interpreted exhaustively, leaving a wealth of valuable information unexploited. In this talk, I will discuss our recently developed method based upon supervised machine learning of X-ray spectra through the development of a deep neural network (DNN) [2]. This DNN is able to predict spectra in less than a second with no input beyond geometric information about the local environment of the absorption site. We predict peak positions with sub-eV accuracy and peak intensities with errors over an order of magnitude smaller than the spectral variations that the model is engineered to capture. I will also discuss challenges and methods used to predict the expected uncertainties.

1. C. J. Milne, T. J. Penfold and M. Chergui, *Coord. Chem. Rev.* **277**, 44-68 (2014)
2. C. D. Rankine, M. M. M. Madkhali, and T. J. Penfold, *J. Phys. Chem. A*, **124**, 4263 (2020)

Host: Jochen Küpper/ CFEL Molecular and Ultrafast Science Seminar