

Robust recognition and exploratory analysis of crystal structures via Bayesian deep learning (canceled)

Monday, 11 April 2022 15:15 (30 minutes)

Due to their ability to recognize complex patterns, neural networks can drive a paradigm shift in the analysis of materials-science data. As a major improvement, we introduce a crystal-structure identification method based on Bayesian deep learning that is robust to structural noise and can treat more than 100 crystal structures. While being trained on ideal structures only, our method correctly characterizes strongly perturbed single- and polycrystalline systems, from both synthetic and experimental resources. Robust crystal classification, principled uncertainty estimates, and exploratory analysis of internal neural-network representations (via unsupervised learning) enable hitherto hindered investigations of noisy atomic structural data.

https://cloud.fhi-berlin.mpg.de:8443/getlink/fiA1s3hPPgAmDotS7GAiqupa/BiGmax_talk_Leitherer_April_11_2022.pdf

Poster title

Primary author: LEITHERER, Andreas (Fritz Haber Institute of the Max Planck Society)

Co-authors: Dr ZILETTI, Angelo (Fritz Haber Institute of the Max Planck Society); Dr GHIRINGHELLI, Luca M. (Fritz Haber Institute of the Max Planck Society)

Presenter: LEITHERER, Andreas (Fritz Haber Institute of the Max Planck Society)

Session Classification: Session I