Contribution ID: **41** Type: **Talk**

Robust recognition and exploratory analysis of crystal structures via Bayesian deep learning (12 min talk + 3 min discussion)

Thursday, 15 April 2021 12:00 (15 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.

Poster title

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