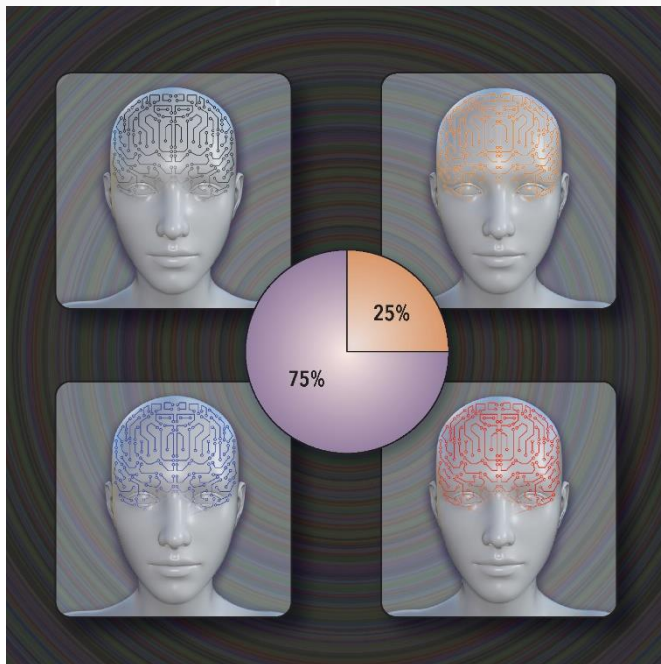


Materials Discovery Through AI-powered Consensus



This image illustrates the result of the voting process by the different AIs in the ensemble. The researcher can use these results inform their further analysis of the x-ray diffraction data to answer their scientific questions.

P.M. Maffettone, L. Banko, P. Cui, Y. Lysogorskiy, M. A. Little, D. Olds, A. Ludwig, A. I. Cooper. Crystallography companion agent for high-throughput materials discovery. *Nat. Comput. Sci.* 1, 290–297 (2021).

Work was performed in part at Brookhaven National Laboratory

Scientific Achievement

Scientists developed an artificial intelligence (AI) ensemble for autonomous characterization of x-ray diffraction (XRD) data and demonstrated its performance on organic and inorganic materials.

Significance and Impact

While automation has accelerated the rate of measurement for materials discovery, the analysis techniques are still time-consuming and error-prone. This study offers researchers a fast classification tool to improve the accuracy of data analysis, while saving time.

Research Details

- Each AI within an ensemble is pre-trained on existing simulated XRD data based on a materials database.
- Ensemble autonomously votes to classify potential material structure solutions based on the measured XRD data.
- Ensemble predicts accurately & knows its uncertainty
- Showed effectiveness across a diverse set of materials, measured at the PDF beamline at NSLS-II.