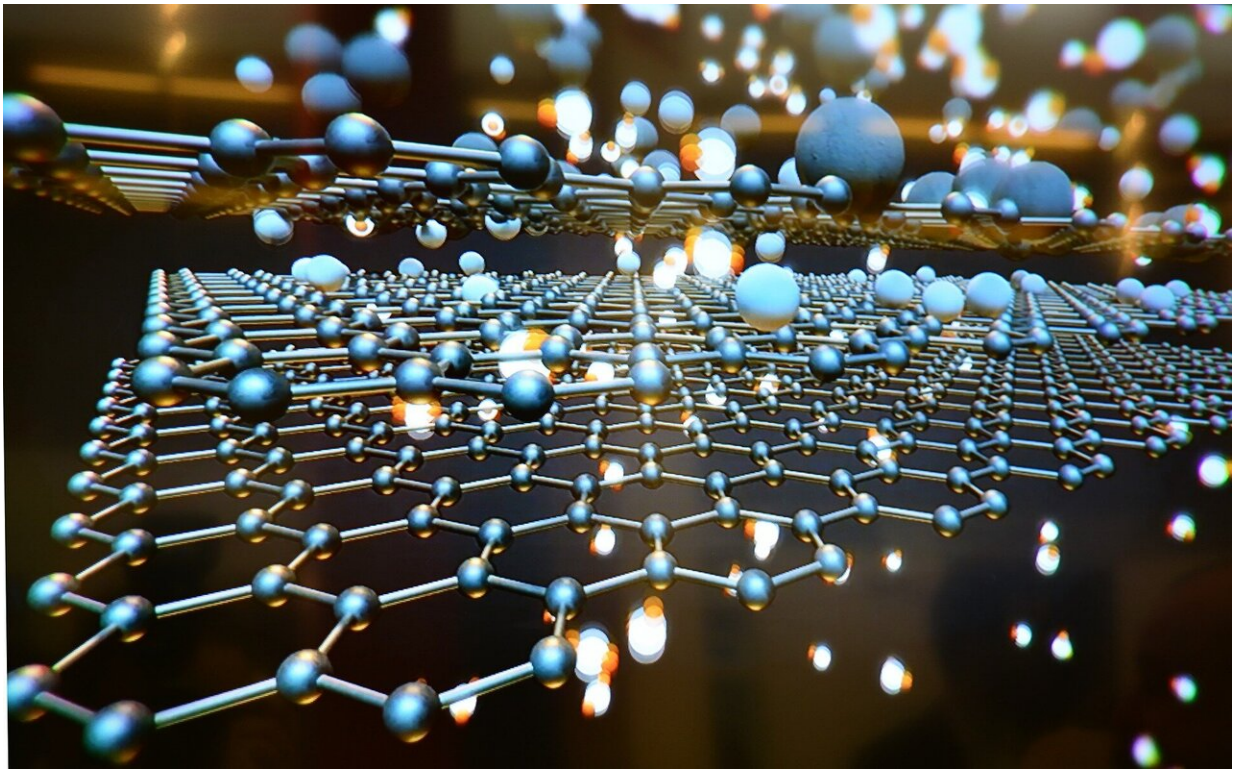
# AI agent helps identify material properties faster

April 20 2021



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Efficient analysis of X-ray diffraction data (XRD) plays a crucial role in the discovery of new materials, for example for the energy systems of the future. It is used to analyze the crystal structures of new materials in order to find out, for which applications they might be suitable. XRD

measurements have already been significantly accelerated in recent years through automation and provide large amounts of data when measuring material libraries. "However, XRD analysis techniques are still largely manual, time-consuming, error-prone and not scalable," says Alfred Ludwig. "In order to discover and optimize new materials faster in the future using autonomous high-throughput experiments, new methods are required."

In a new publication in *Nature Computational Science*, a team headed by Dr. Phillip M. Maffettone (currently at National Synchrotron Light Source II in Upton, U.S.) and Professor Andrew Cooper from the Department of Chemistry and Materials Innovation Factory at the University of Liverpool, and Lars Banko and Professor Alfred Ludwig from the Chair of Materials Discovery and Interfaces and Yury Lysogorskiy from the Interdisciplinary Centre for Advanced Materials Simulation shows how artificial intelligence can be used to make XRD data analysis faster and more accurate. The solution is an AI agent called Crystallography Companion Agent (XCA), which collaborates with the scientists. XCA can perform autonomous phase identifications from XRD data while it is measured. The agent is suitable for both organic and inorganic material systems. This is enabled by the large-scale simulation of physically correct X-ray diffraction data that is used to train the algorithm.

## Expert discussion is simulated

What is more, a unique feature of the agent that the team has adapted for the current task is that it overcomes the overconfidence of traditional neuronal networks. Such networks make a final decision even if the data doesn't support a definite conclusion, whereas a scientist would communicate their uncertainty and discuss results with other researchers. "This process of decision-making in the group is simulated by an ensemble of neural networks, similar to a vote among experts," explains

Lars Banko. In XCA, an ensemble of neural networks forms the expert panel, so to speak, which submits a recommendation to the researchers. "This is accomplished without manual, human-labeled data and is robust to many sources of experimental complexity," says Banko.

XCA can also be expanded to other forms of characterisation such as spectroscopy. "By complementing recent advances in automation and autonomous experimentation, this development constitutes an important step in accelerating the discovery of new materials," concludes Alfred Ludwig.

**More information:** Phillip M. Maffettone et al. Crystallography companion agent for high-throughput materials discovery, *Nature Computational Science* (2021). DOI: 10.1038/s43588-021-00059-2

Provided by Ruhr-Universitaet-Bochum