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Solving atomic structures by combining analysis of PDF pattern with DFT calculations in machine learning enhanced global optimization

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Determination of crystal structures of nano-crystalline, or amorphous compounds is a great challenge in solid states chemistry and physics. Structural analysis using atomic pair distribution function (PDF) of X-ray or neutron total scattering data has the potential to become a very efficient method in this field. Unfortunately, for real-space structure refinements using this method, an initial starting model for the atomic positions is needed, but not available in many cases. To solve this problem, we have recently introduced an algorithm [1, 2] that is able to determine the crystal structure of an unknown compound by means of an on-the-fly trained machine learning (ML) model that combines density functional calculations (DFT) with comparison of calculated and measured PDFs for global optimization. The PDF might be obtained from X-Ray or neutron scattering Data or a combination of both. In our previous work, we showed, that the algorithm is able to predict stacking disorder in layered compounds and even meta-stable point defects in spinel structures with particle sizes below 4 nm. In an ongoing study, we are focusing on even smaller particle sizes and are now able to present all-atom structure models of supported and unsupported particles down to the 1 nm range.

[1] M. Kløve, S. Sommer, B.B. Iversen, B. Hammer, W. Dononelli; *Machine learning based approach for solving atomic structures of nanomaterials combining pair distribution functions with density functional theory*, Advanced Materials **35**, 2208220 (2023)
[2] W. Dononelli; *Das Experiment direkt in die quantenchemische Modellierung einbeziehen*, Bunsen Magazine **6**, 204-207 (2023)

Primary author: Dr DONONELLI, Wilke (Universität Bremen)

Presenter: Dr DONONELLI, Wilke (Universität Bremen)

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