3DED-QCR: THREE-DIMENSIONAL ELECTRON DIFFRACTION MEETS QUANTUM CRYSTALLOGRAPHY

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PROJECT GOAL

The aim of the project is to improve the determination of crystal structures of nanocrystals. Knowing the crystal structure of an investigated material is very important for understanding its properties. To get the crystal structures from very small single crystals (smaller than one micrometre), a method called three-dimensional electron diffraction (3D ED) must be used. However, the analysis of electron diffraction data is complicated and it still poses a number of challenges. One of them is the possibility to include in the analysis the effect of interactions between the atoms in the crystal structure. This part of crystal-structure analysis belongs to the area of quantum crystallography. The goal of this project is to connect the world of 3D ED and quantum crystallography, and make it possible to access the quantum-crystallographic information from very small crystals.

REASONS FOR CONDUCTING THE RESEARCH

Quantum crystallography provides a wealth of information about the materials we use in everyday life, from metal alloys and ceramic materials all the way to pharmaceuticals and biomolecules. It allows us to understand, how and why the materials have the properties they have. It also allows us to determine the crystal structure with higher accuracy. Experimental determination of these properties is crucial for validation of theoretical calculations and it is indispensable in cases where the theory still does not provide reliable results. We want to make this information accessible for materials for which it was not accessible so far.

HOW THE RESEARCH WILL BE CONDUCTED

The project will be conducted in collaboration between groups at the Warsaw University and at the Institute of Physics of the Czech Academy of Sciences at Prague. The Warsaw group has rich experience with quantum crystallography, while the Prague group provides the know-how about accurate structure analysis using the 3D ED method. The first steps in the research will be the collection of very high-quality diffraction data, and comparing them with theoretical calculations. Once a good agreement is confirmed, we will proceed to modifying the software needed to extract the chemical information to work with electron diffraction data. Two models will be tested – a so called TAAM (transferable aspherical atom model), where the interatomic interactions are determined using theoretical calculations and used to improve the description of experimental data, and the multipolar refinement method, which allows an independent determination of the interatomic interaction purely from experimental data.

MAIN EXPECTED RESULTS

The key result will be a set of methods and software tools for performing quantum-crystallographic structure determination on electron diffraction data. These tools will be made available for other scientists to allow them to obtain better results in their research. We also plan to apply the developed methods to interesting scientific problems.