Seeing Beyond Imaging: The Power of Electron Diffraction

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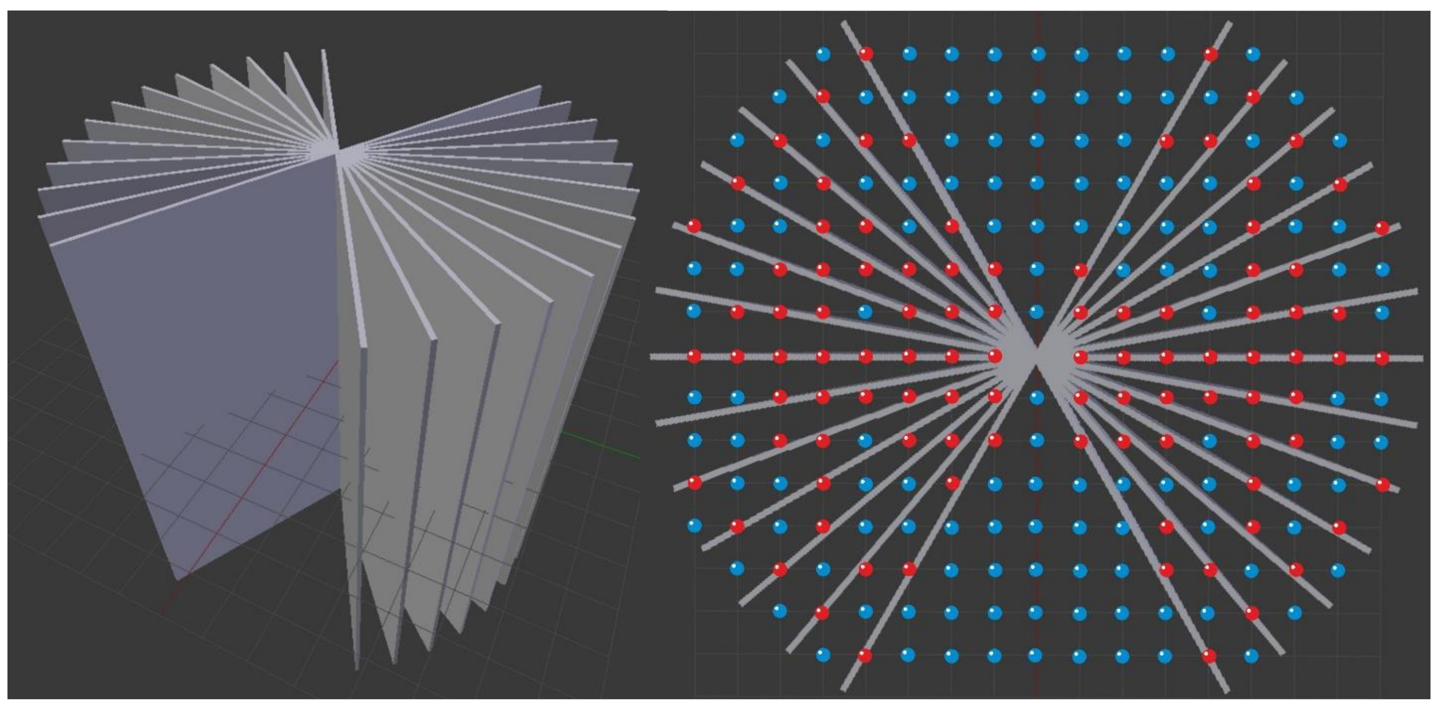
Electron diffraction has traditionally played a supporting role in TEM, primarily for pre-aligning crystals for high-resolution imaging. However, with advancements in 3D data acquisition over the past decade, electron diffraction has evolved into a powerful standalone technique for structural characterization. The combination of high data resolution, large data volumes, and significantly reduced electron dose has expanded its applications across materials science, chemistry, and structural biology.

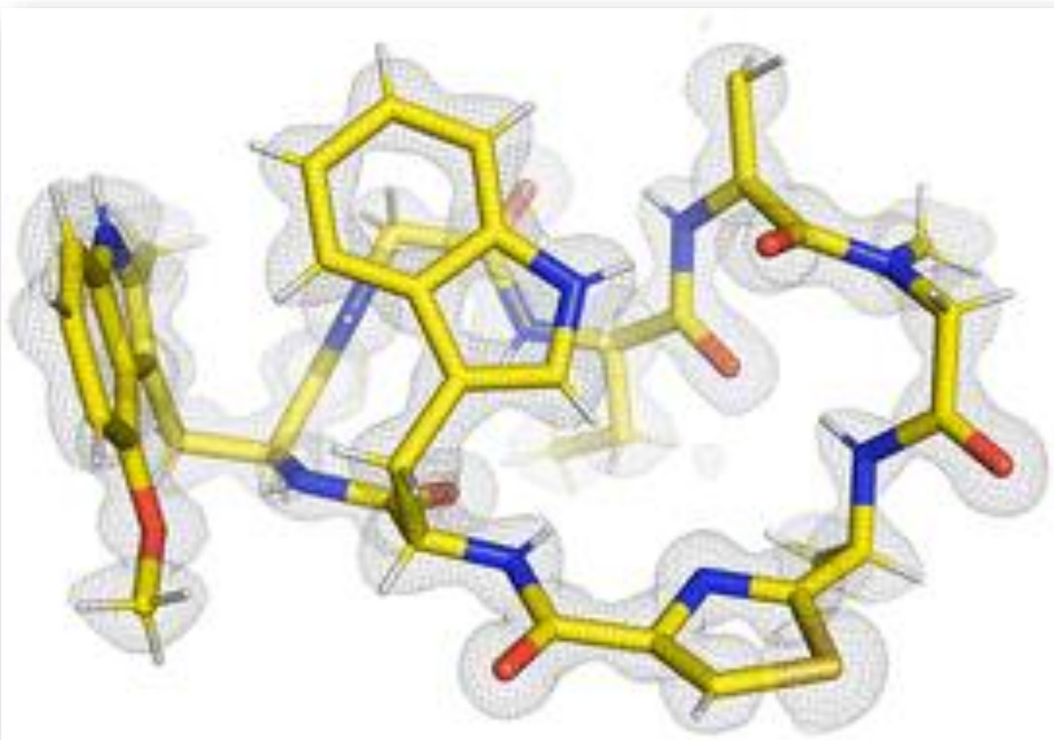
How it is done: 3D ED

The concept of 3D ED is based on recording a series of 2D electron diffraction patterns (tilt series) while rotating a crystal around the primary goniometer axis. This axis is not aligned with any specific crystallographic direction of the crystal. Two different data collection geometries can be used: stepwise acquisition, assisted by conical precession, and continuous rotation (later rebranded as MicroED), which represents a form of “linear precession.” Currently, research in 3D ED data collection focuses primarily on developing methods to reduce electron dose during acquisition, including various strategies for crystal tracking.



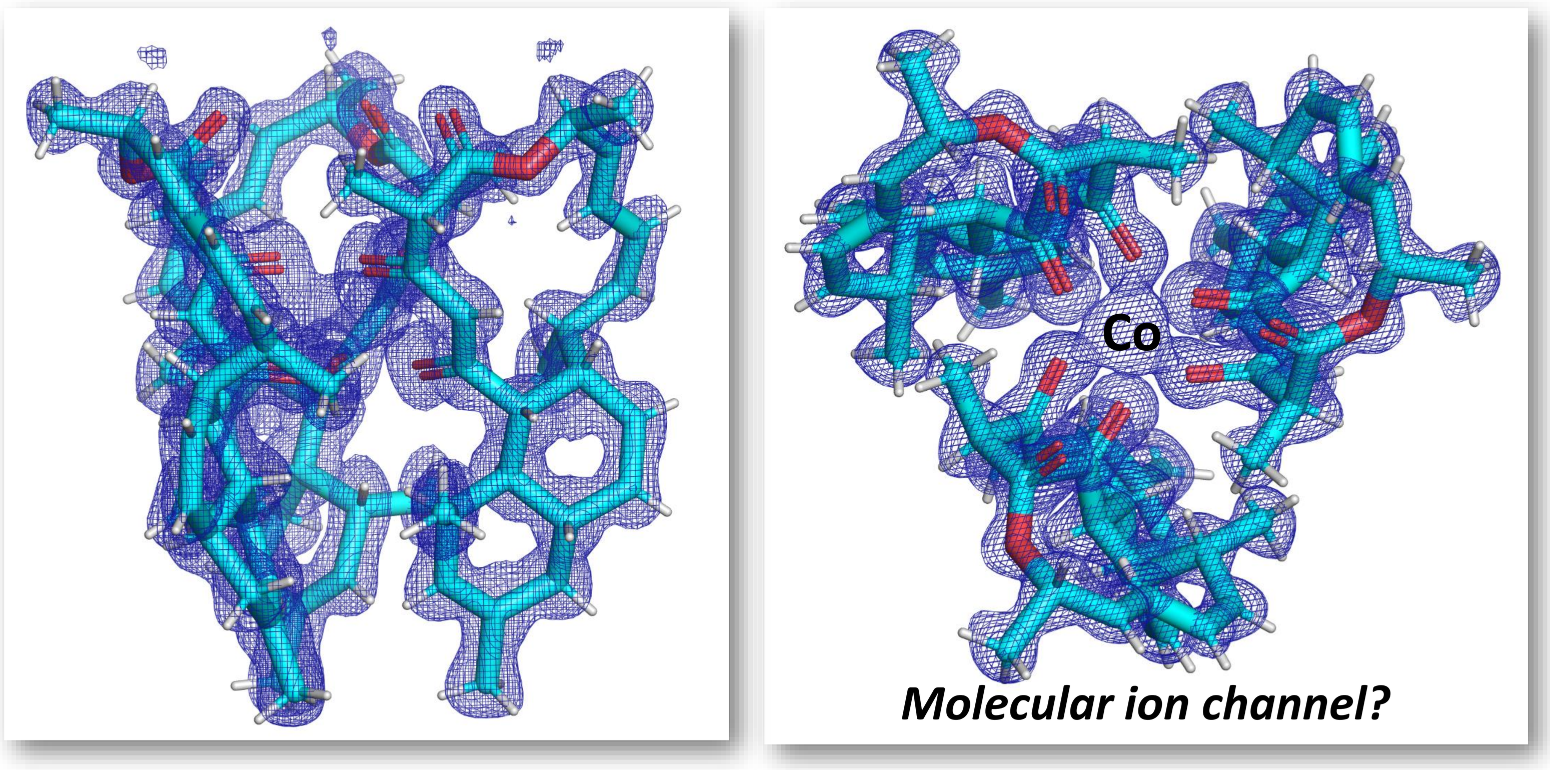
Applications: crystal structure determination of beam sensitive organic compounds

Natural product: Argyrin-D



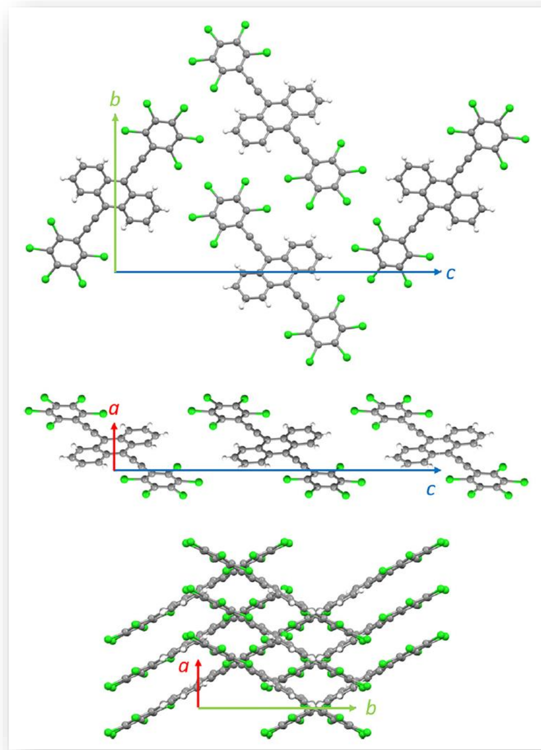
Gorelik, et al., 2022. CrystEngComm, 24, 5885.

Natural product: [Chlorotonil] Dehalogenil Co complex



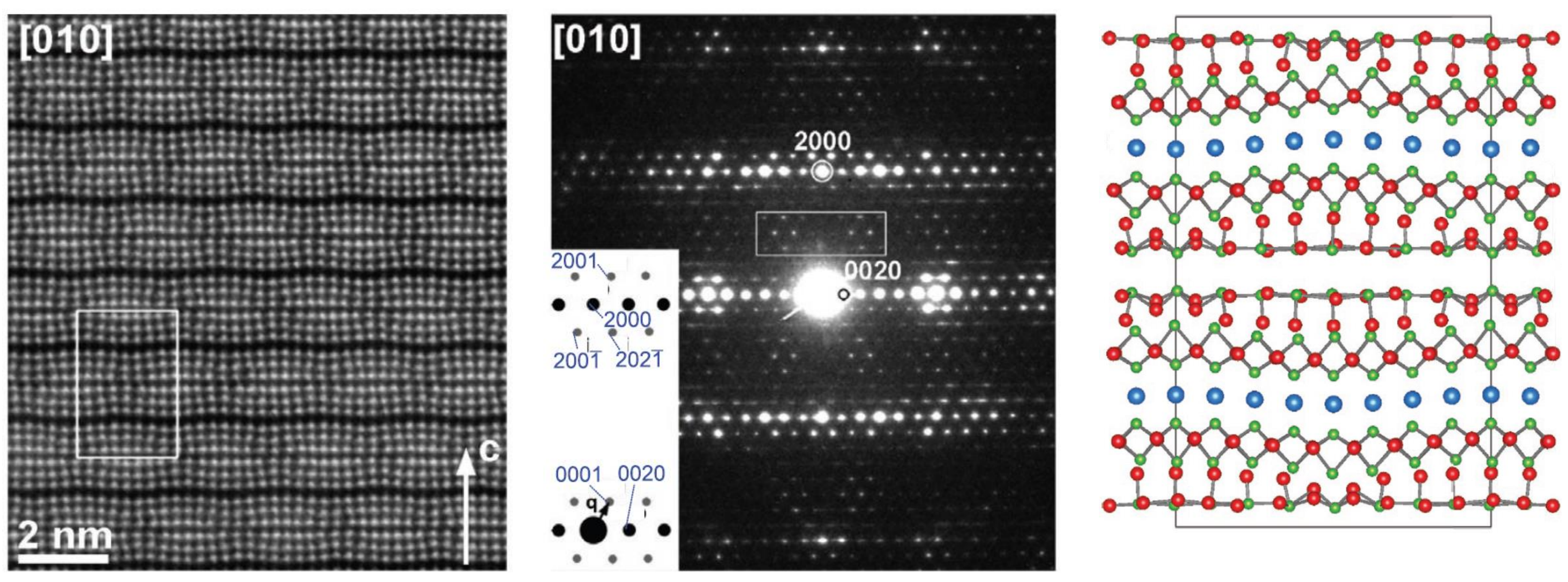
Deschner et al., 2024 Cell Chemical Biology, submitted

Photovoltaics



Gorelik et al., 20203, Z. Kristallogr. 238, 253

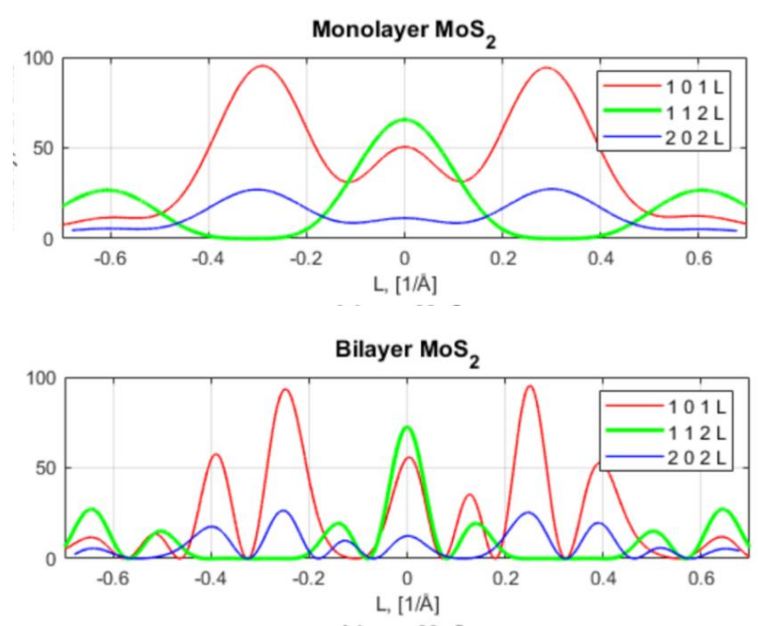
Complex functional materials: $Bi_{12}O_{17}Cl_2$ superstructure

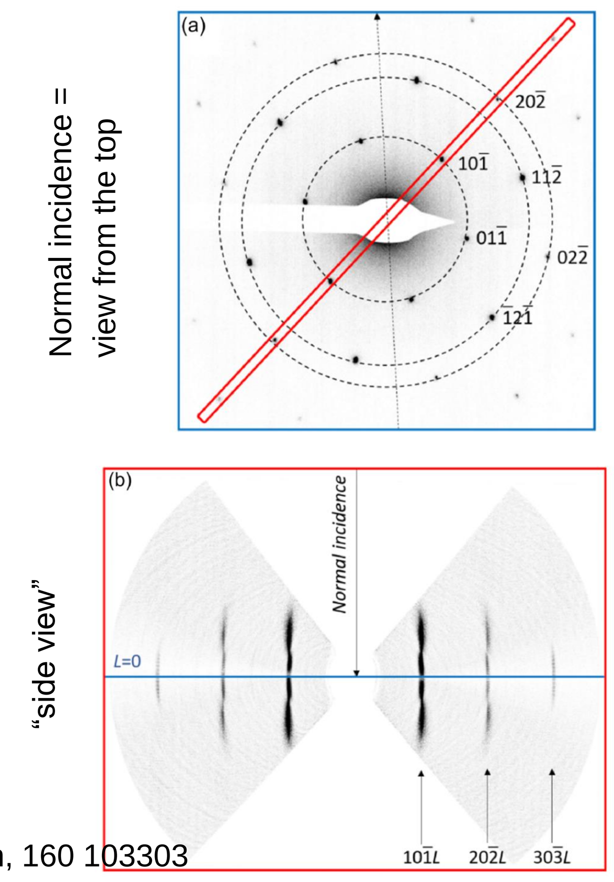


$Bi_{12}O_{17}Cl_2$ with a Sextuple Bi—O Layer Composed of Rock-Salt and Fluorite Units and its Structural Conversion through Fluorination to Enhance Photocatalytic Activity

Kato et al., Adv. Funct. Mater. 2022, 2204112

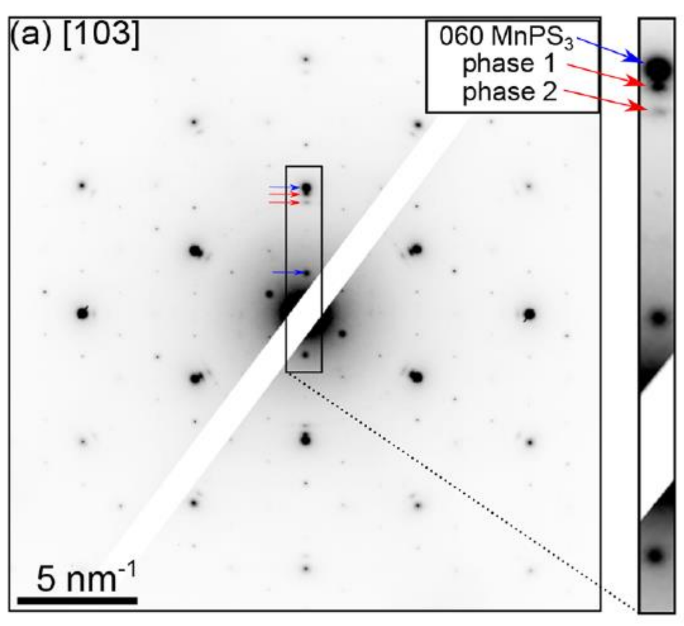
2D crystals: graphene, TMDs – structural information along z





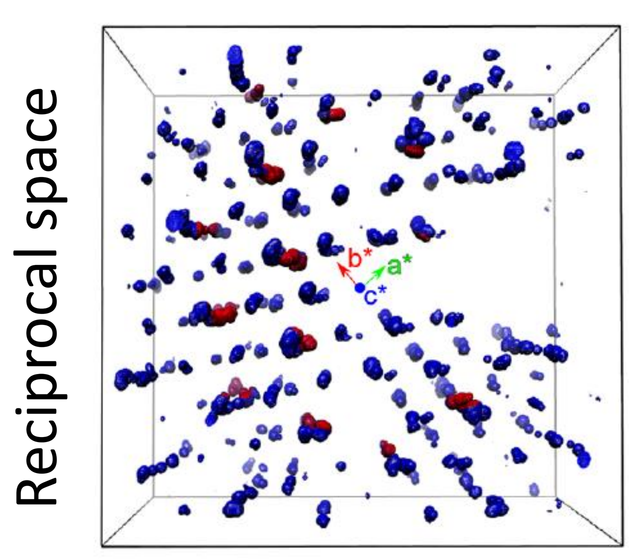
Gorelik et al., 2021. Micron, 146, 103071, Köstner et al., 2022. Micron, 160 103303

3D Orientation relationship between the matrix phase and precipitates



Storm et al., 2023. ACS Nano, 17, 4250

Growth of MnS nanocrystals within $MnPS_3$ after electron irradiation

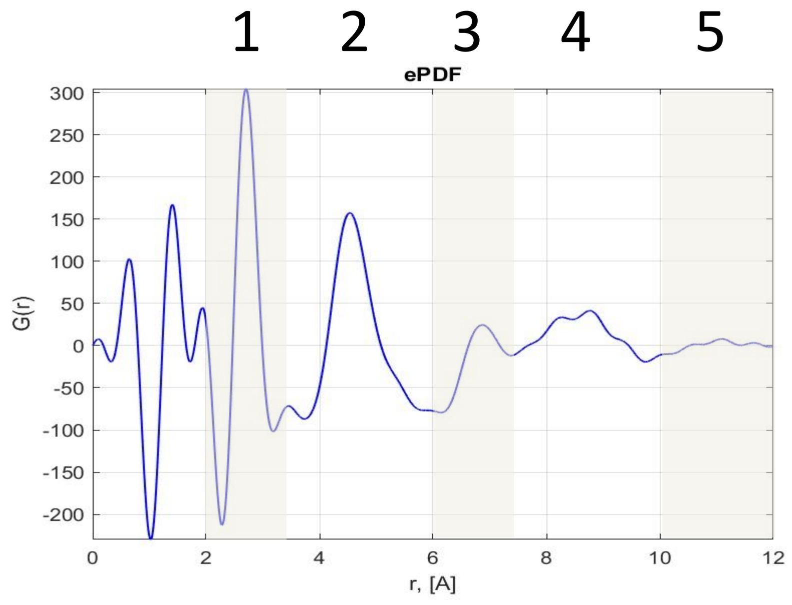


Blue – matrix, red – precipitates

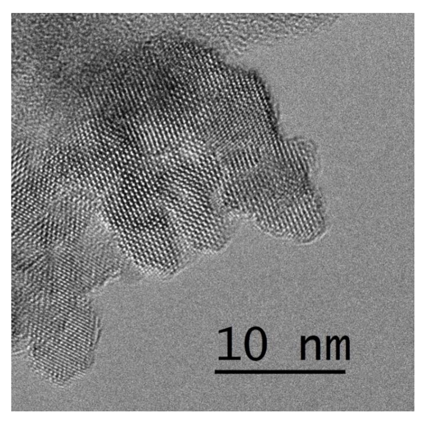
Electron Pair Distribution Function – beyond crystallinity

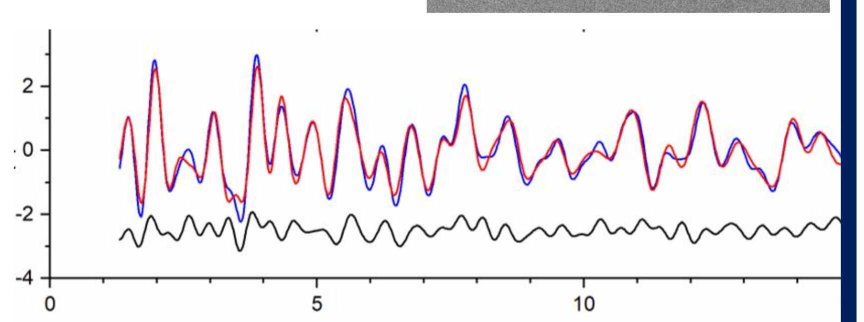
Vitrified water:
5 coordination shells

1 2 3 4 5



Nanocrystalline anatase: quantification of ePDF, refinement





Gorelik et al., 2019. Acta Cryst. B75, 532