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Combining Reverse Monte Carlo Analysis of X-ray Scattering and Extended X-ray absorption Spectroscopy

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Extended X-ray absorption fine structure (EXAFS) spectra contain information about the local, molecular type structure, whereas (X-ray) diffraction (XRD) data reveal the periodic structure or long-range order (crystal structure) of materials. Variations in local and periodic structure greatly influence materials properties and related applications. However, data analysis often is performed independently for EXAFS spectra and diffraction data even if measured simultaneously.
RMC simulations enable the analysis of X-ray scattering (XS) data as well as EXAFS spectra data via partial pair distribution (pPDF) functions obtained from a physical, structural model. In case of nanoparticles and scattering data this approach suffers from the termination of the pPDF's due to the finite size of the particles. This produces artifacts in the computed scattering intensity due to the long-range probing distance of scattering which are eliminated using the Debye scattering equation (DSE) [1, 2]. Simultaneous refinement of XS data and EXAFS spectra of small nanoparticles are thus enabled using a mutual structural model. This method allows the self-consistent extraction of complementary information on local structure contained in EXAFS and long-range order in XS data. However, refinement of raw diffraction data for crystals of larger domain size (larger than about 10 nm or 50.000 atoms) are difficult. A Rietveld code embedded into the RMC code and feedback of the essential structural information between both refinement paths enables the coupled refinement of diffraction and EXAFS data are in this case [3].

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[2] V. Mackert, T. Winter, S. Jackson, R. Kalia, A. Levish, S. Lukic, J. Geiss, and M. Winterer, Very Small Nanocrystalline Tin Dioxide Particles: Local-, Crystal-, and Micro-Structure, J. Phys. Chem. C 127 (2023) 17389–17405, 16p.; doi.org/10.1021/acs.jpcc.3c02110
[2] M. Winterer, Coupling Rietveld refinement of X-ray diffraction data and reverse Monte Carlo analysis of extended X-ray absorption fine structure spectra, J. Mat. Res. 40 (2025) 649-661; doi.org/10.1557/s43578-025-01545-3

Presenter: Prof. WINTERER, Markus (University of Duisburg-Essen)

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