MS26 Quantum mechanical models for dynamics and diffuse scattering

MS26-05
Diffuse scattering from crystals - quantifying the contribution of lattice dynamcis and disorder
B. Wehinger [1]
[1]ESRF - The European Synchrotron - Grenoble (France)

Abstract
I will present quantitative modelling of diffuse scattering intensities from first principles including contributions from lattice dynamics and disorder and illustrate its application to quantum materials. I will show how high-precision measurements of diffuse scattering intensities together with a rigorous data analysis allow for the determination of the full elasticity tensor [1]. Modelling diffuse scattering from first principles allows to understand unusual features in the distribution of scattering intensities and allows for quantitative statements on the microscopic origin [2]. Finally, I will show how the application of diffuse scattering to quantum materials allow us to discover new fundamental phenomena at the forefront of quantum-many-body physics [3].

References
[1] Björn Wehinger, Alessandro Mirone, Michael Krisch and Alexeï Bosak, Full Elasticity Tensor from Thermal Diffuse Scattering, Phys. Rev. Lett. 118, 035502 (2017).
[2] Björn Wehinger, Dmitry Chernyshov, Michael Krisch, Sergey Bulat, Victor Ezhov and Alexeï Bosak, Diffuse scattering in Ih ice, J. Phys.: Condens. Matter 26 265401 (2014).
[3] Sándor Tóth, Björn Wehinger, Katharina Rolfs, Turan Birol, Uwe Stuhr, Hiroshi Takatsu, Kenta Kimura, Tsuyoshi Kimura, Henrik M. Rønnow and Christian Rüegg, Electromagnon dispersion probed by inelastic X-ray scattering in LiCrO2, Nat. Comm. 7, 13547 (2016).

Diffuse scattering in ice Ih [2]