



Contribution ID: 19

Type: **Talk**

## Sensitivity of thermal diffuse scattering to correlated disorder

*Tuesday, 15 March 2022 14:20 (20 minutes)*

We show that thermal diffuse scattering is sensitive to correlated disorder. We utilise the family of disordered rocksalts  $\text{KBr}_{1-x}\text{Cl}_x$  as our model system and analyse the experimentally observed single-crystal X-ray diffuse scattering. Using supercell lattice dynamical calculations we explicitly account for the changes to the dynamics of a system due to correlated disorder.

**Primary author:** SCHMIDT, Ella Mara

**Co-authors:** Mr BULLED, Johnathan M. (Inorganic Chemistry, University of Oxford ); Prof. GOODWIN , Andrew L. (Inorganic Chemistry, University of Oxford ); Dr MINELLI, Arianna (Inorganic Chemistry, University of Oxford ); Mrs THOMAS, Sofia (Inorganic Chemistry, University of Oxford )

**Presenter:** SCHMIDT, Ella Mara

**Session Classification:** Advanced Structure Analysis II

**Track Classification:** Main conference: Advances in Methods, Instrumentation and Data Analysis