Contribution ID : **106** Type : **Oral**

Atomistic modelling as a complementary tool for diffraction studies

Thursday, 12 November 2020 10:45 (20)

Diffraction experiments typically provide clear picture of a crystal structure and basis for understanding material properties. However, for materials with high static or dynamic disorder and/or weakly occupied atomic sites, the diffraction data reflecting space- and time-averaged state may struggle to distinguish several alternative models yielding similar $\chi 2$. In that case, atomistic modelling may help not only to identify the more energetically stable configuration but also provide insights into the mechanism of its formation. I will present several recent examples of studies of disordered oxygen and proton ionic conductors, where empirical and ab initio static and geometry optimisation calculations and molecular dynamics simulations not only helped to validate neutron diffraction analysis but also revealed the mechanism driving the disorder.

Speakers Gender

Male

Level of Expertise

Expert

Do you wish to take part in the poster slam

No

Primary author(s) : AVDEEV, Max (Australian Nuclear Science and Technology Organisation, Australian Centre for Neutron Scattering)

Presenter(s) : AVDEEV, Max (Australian Nuclear Science and Technology Organisation, Australian Centre for Neutron Scattering)

Session Classification : Chemistry & Crystallography

Track Classification : Chemistry & Crystallography