

Atomistic modelling as a complementary tool for diffraction studies

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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 χ^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.

Level of Expertise

Expert

Speakers Gender

Male

Do you wish to take part in the poster slam

No

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