

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 data of poor quality or in case of materials with high static or dynamic disorder and/or weakly occupied atomic sites, diffraction may struggle to distinguish several alternative models yielding similar χ^2 . In that case, atomistic modelling may be very useful to identify the correct model. I will present several recent examples of studies of disordered oxide-ion and cation 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.