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, e.g. ionic conductors, 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 oxide-ion and proton conductors, where *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.

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