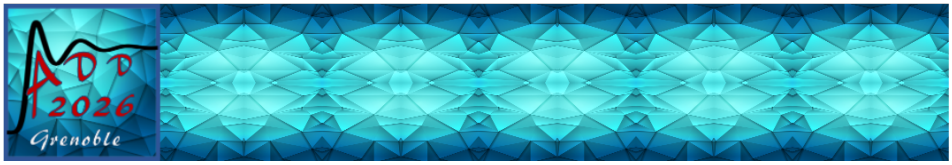

Contribution ID: **7** Type: **Invited**

EPSR & Dissolve - Data-driven structural modelling of total scattering data

The study of disordered materials such as liquids and glasses through neutron or x-ray techniques presents an interesting challenge since, due to the presence of only local order (< 1 nm) in these materials, only diffuse scattering prevails. Searching for, or generating model analogues that match this "order in disorder" present in the structure of real systems is normally required to make any kind of scientific interrogation. This is the goal of the Empirical Potential Structure Refinement (EPSR) [1] and Dissolve [2] codes.

Both EPSR and Dissolve rely on a full, atomistic simulation (Monte Carlo and/or molecular dynamics) of a target system and its constituent molecules and moieties within the context of a "realistic" forcefield describing the interactions between atoms. While simulations utilising off-the-shelf forcefields typically do not reproduce experimentally-measured structure factors, they act as a useful starting point for further refinement. Critically, the provision of experimental scattering data allows both codes to modify the interatomic potentials provided and drive the simulated system towards better agreement with the real-world one. This data-driven approach to the modelling of total-scattering data has successfully been applied to a multitude of disordered systems covering liquids, liquid mixtures, and glasses, and is increasingly being used to study complex disordered materials such as gases and liquids confined in porous materials, polymers in solution, and self-assembled systems such as aqueous micelles.

Here I will give an overview of the techniques and approaches involved, their advantages, limitations and challenges, and discuss some real-world examples.

[1] Soper, *Mol. Phys.* **99**, 1503 (2001)
[2] Youngs, *Mol. Phys.* **117**, 3464 (2019)

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Session Classification: Tutorial introductions