Neutron PDF–Constrained Atomic Modelling of Amorphous Solid-State Electrolytes

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Abstract

Determining realistic 3D atomic structures of amorphous solid-state electrolytes (SSEs) from neutron pair distribution function (PDF) data is a challenging inverse problem.[1] Many distinct atomic configurations can reproduce similar pair-correlation signatures, and PDF-based structural inference for disordered materials is generally non-unique.[2] Identifying physically meaningful structural motifs from PDF data remains challenging even when many candidate fits are available.[3] To address this, we are developing a general workflow for amorphous structure generation and key-property prediction under experimental PDF constraints. Our framework takes target PDF, composition, and density as inputs and outputs a vetted ensemble of amorphous candidates that simultaneously satisfy PDF matching, density constraints, and physical plausibility, enabling downstream structure–property analysis and machine-learning force-field refinement.

References

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[2] A. Pandey, P. Biswas, D. A. Drabold, Scientific Reports 6 (2016) 33731.
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Figures

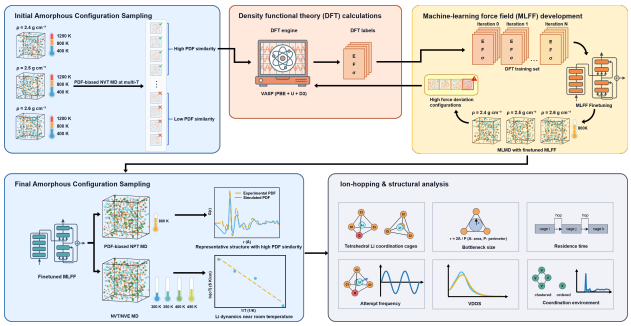

Figure 1. Schematic diagram of the workflow for amorphous structure generation and key-property prediction under experimental PDF constraints