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Data Agent-Driven Construction of High-Quality Cross-Facility Diffraction Datasets

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Experimental data generated by scientific facilities such as synchrotron radiation and neutron sources provide a fundamental resource for scientific research. With the deepening integration of massive scientific data and artificial intelligence (AI) technologies, the paradigm of scientific inquiry is undergoing a transformative shift. This evolution places higher demands on the integrated management of data systems in large-scale facilities and the AI-ready datasets processing of simulated and experimental data. In the field of materials science, X-ray diffraction (XRD) and neutron powder diffraction (NPD) each offer unique and complementary advantages in resolving crystal structures. However, effectively integrating these two types of heterogeneous data remains a significant technical challenge. To address this issue, we have developed a cross-facility data agent designed to unify and coordinate diffraction data streams from synchrotron radiation and neutron sources. This agent establishes a closed-loop workflow that encompasses simulated data generation and joint refinement of experimental data. The core mechanism involves systematically minimizing the discrepancy between simulated and experimental data, thereby achieving effective alignment of simulated data with experimental observations. The high-quality cross-facility diffraction datasets constructed through this approach provide a reliable data foundation for training AI models in crystal structure prediction, while also opening up a new technical pathway for accelerating research on structure–property relationships in materials.

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