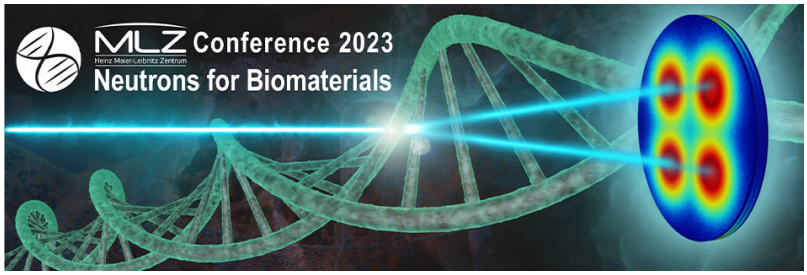


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# Bridging Direct and Reciprocal Space: Using Molecular Dynamics Simulations and Scattering Experiments to Study Biological Membranes

Biological membranes are primarily composed of phospholipid-based bilayers, which serve as their fundamental structural elements. In this study, we present an approach that combines experimental neutron scattering data with molecular dynamics (MD) simulations to investigate phospholipid membrane systems. Neutron and X-ray reflectometry measurements are determined by the scattering length density profile in real space. However, this profile is often challenging to retrieve unambiguously from the data alone. MD simulations predict these density profiles, but they require experimental validation. By cross-validating scattering data and MD results, we can simultaneously address both issues. We'll present the strengths and weaknesses of each technique. The complementarity between scattering methods and MD simulations is remarkable, as it not only bridges the gap between direct and reciprocal space, but also provides unique insights into each other's limitations. To facilitate these insights, we have created a new software program named Made2Reflect, which directly calculates neutron and X-ray small-angle scattering and reflectivity patterns from MD simulation trajectories.

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