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Nanoscale Structure of Lipid Bilayers Revealed by In-Silico and Experimental Small Angle Neutron Scattering[1] MITCHELL DORRELL, Department of Physics and Astronomy, University of Delaware, FRED HEBERLE, Biology and Soft Matter Division, Oak Ridge National Laboratory, JOHN KATSARAS, Biology and Soft Matter Division, Oak Ridge National Laboratory, and Department of Physics and Astronomy, The University of Tennessee, EDWARD LYMAN, Department of Physics and Astronomy and Department of Chemistry and Biochemistry, University of Delaware — Through the combination of simulations and numerical analysis with small angle neutron scattering, we probe the lateral organization of lipid bilayer mixtures. Small Angle Neutron Scattering (SANS) is an excellent complement to optical techniques, as it reveals molecular scale structural details without fluorescent probes. On its own, however, SANS is not sufficient to determine the organization of the membrane. We therefore take a two-pronged approach, comparing molecular dynamics simulations of ternary mixtures to experimental data obtained for the same mixtures. In-silico neutron scattering experiment intensities on simulated membranes are fitted to the experimental data, simultaneously validating the simulation data and providing a molecular scale model of the experimental system. In this way, the transverse variation in scattering length density across the bilayer which, under fully deuterated solvent, is much more significant than lateral contributions is used to infer lateral structure.

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Mitchell Dorrell
University of Delaware

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