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A Computational Approach to Model Neutron Scattering Data from Lipid Bilayers¹ JAN-MICHAEL CARRILLO, JOHN KATSARAS, BOBBY SUMPTER, RANA ASHKAR, Oak Ridge National Laboratory — The successful interpretation of multimodal characterization experiments of soft materials, such as lipid membranes in complex environments, requires the use of efficient computer simulation protocols, which are intended to supplant the spatially and temporally limited experimental measurements of membrane structures and dynamics. Here, we describe our coarse-grained MD simulation approach that can mimic neutron scattering data from unilamellar lipid vesicles over a range of bilayer rigidity. Specifically, we simulate vesicle form factors and membrane thickness fluctuations determined from small angle neutron scattering (SANS) and neutron spin echo (NSE) experiments, respectively. Our simulations accurately reproduce trends from experiments and lay the groundwork for investigations of more complex membrane systems.

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