What's so special about cholesterol? Integrating simulations and IXS to identify collective modes in lipid membranes

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The membranes that enclose our cells are made of amphiphiles called lipids, which assemble into a bilayer structure to form a semipermeable barrier between the extracellular and intracellular spaces. The structural parameters of lipid bilayers — the thickness, area per molecule, the orientation of the director — have long been studied by static scattering of x-rays and neutrons, in order to determine how continuum elastic properties emerge from molecular level interactions. Now, recent advances in sources and detection have opened a new meV-IXS window onto membrane structure and dynamics. When integrated with molecular dynamics simulations, meV-IXS data reveal psec to nsec collective dynamics of membranes that are inaccessible by any other technique. A series of simulations and experiments on membranes containing varying amounts of cholesterol show how the dynamic response of membranes depends on this very special lipid, which makes up roughly 30% by mole of our membranes, and which simultaneously fluidizes and orders lipid bilayers.