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**Investigation of Membrane Proteins Dynamics from MD Simulations. Connection to Inelastic Scattering Techniques.** M. Tarek, B. Maigret, C. Chipot, F. Dehez, W. Treptow. Equipe de Dynamique des Assemblages Membranaires, UMR 7565, CNRS- Univ. Henri-Poincaré, Nancy, FRANCE.

Function of membranes and membrane proteins depend on their dynamics and relaxation behavior. These may be in principle probed using -neutron and x-ray- scattering techniques, yet, inelastic data on membrane proteins are very scarce, and still difficult to interpret. In the past we have shown that, combined with experiments, Molecular Dynamics (MD) simulations are able of providing exquisite details about the dynamics of membranes, that of globular proteins and of their associated hydration-water (1). We use here state of the art simulation techniques to perform *in silico* (inelastic and elastic) neutron and x-ray scattering measurements on membrane proteins. We will discuss in particular the appropriate experimental conditions allowing to extract the maximum information from scattering techniques as well as the expected insight from such measurements.

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