

Hydration coupled dynamics in biological macromolecules studied by inelastic neutron and X-ray scattering

BELLISSENT-FUNEL M.-C.

Laboratoire Léon Brillouin (CEA-CNRS), CEA-Saclay, 91191 Gif-sur-Yvette Cedex,
mcbel@llb.saclay.cea.fr

It is well known that water plays a major role in the stability and catalytic function of biomolecules. Both the effect of hydration water on the dynamics of biomolecules (1-2) and the effect of biomolecules on the dynamics of water have been studied using inelastic neutron (3-4) and X-ray scattering (5). Single particle dynamics in biomolecules has been studied using incoherent inelastic neutron scattering which is a unique technique to study diffusive motions of protons in a time scale from subpicoseconds to nanoseconds. In this paper, we present results obtained on hydrated powders of proteins (C-phycoerythrin, parvalbumin) (1-2). Knowledge of collective density fluctuations of hydrocarbon chains in lipid bilayers is essential for understanding some aspects of biological functions of natural membranes. We will show the advance of inelastic X-ray scattering in this field and report on recent results on fully hydrated phospholipid bilayers (5). Some comparison will be done with results of experiments by coherent inelastic neutron scattering on a hydrated protein (2).

References

- [1] - J.-M. Zanotti, Ph-D Thesis, Saclay, 1997; J.-M. Zanotti, M.-C. Bellissent-Funel and J. Parello, *Hydration-coupled dynamics in proteins studied by neutron scattering and NMR. The case of the typical EF-hand calcium-binding parvalbumin*, *Biophys. J.*, **76**, 2390 (1999).
- [2] - S. Dellerue, Ph-D Thesis, Saclay, 2000, S. Dellerue, A. Petrescu, J.C. Smith, S. Longeville and M.-C. Bellissent-Funel, *Collective dynamics of a photosynthetic protein probed by neutron spin-echo spectroscopy and molecular dynamics simulation*, *Physica B*, **276-278**, 514-515 (2000).
- [3] - M.-C. Bellissent-Funel, J.-M. Zanotti and S.H. Chen, *Slow dynamics of water molecules on surface of a globular protein*, *Faraday Discussion*, **103**, 281 (1996).
- [4] - S. Dellerue and M.-C. Bellissent-Funel, *Relaxational dynamics of water molecules at protein surface*, *Chem. Phys.* **258**, 315-325 (2000).
- [5] - S. H. Chen, C.Y Liao, H.W. Huang, T.M., Weiss, M.-C Bellissent-Funel, F. Sette, *Collective dynamics in fully hydrated phospholipid bilayers studied by inelastic X-ray scattering*, *Physical Review Letters* **86**, 740-743 (2001).