Probing protein melting by atomic fluctuations

Marina Katava*†, Fabio Sterpone2, Simone Capaccioli3, and Alessandro Paciaroni4

1Laboratoire de biochimie théorique (LBT) – CNRS : UPR9080, Université Paris VII - Paris Diderot –
13 Rue Pierre et Marie Curie 75005 PARIS, France
2Laboratoire de Biochimie Theorique – CNRS : UPR9080 – France
3University of Pisa, Department of Physics – Italie
4University of Perugia, Department of Physics – Italie

Résumé

The interplay between protein rigidity and flexibility on different length- and time scales
is an important factor in stability at high temperatures. The present work employs Molecular
Dynamics simulations in order to investigate the temperature dependence of atomic fluctua-
tions in a Lysozyme protein embedded in different environments. We show, according to the
Lindemann criterion, that the atomic fluctuations can probe protein melting temperature.
Indeed, the fluctuations of hydrogen atoms of the Lysozyme in a dilute water solution, glyc-
erol solution, and in dehydrated powder are shown to be similar approaching different melting
temperatures of respective systems. Simulation results are in good agreement with Elastic
Incoherent Neutron Scattering experiments of the simulated systems.

Mots-Clés: molecular dynamics, proteins, Lindemann criterion

*Intervenant
†Auteur correspondant: marina.katava@gmail.com