Probing protein melting by atomic fluctuations

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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 fluctuations 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, glycerol 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

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