ENERGY TRANSPORT IN PEPTIDES STUDIED BY NUMERICAL SIMULATIONS

LABORATORY : Institut Lumière Matière

LEVEL : M1
TEAM(S) : MMCI
THEOCHEM

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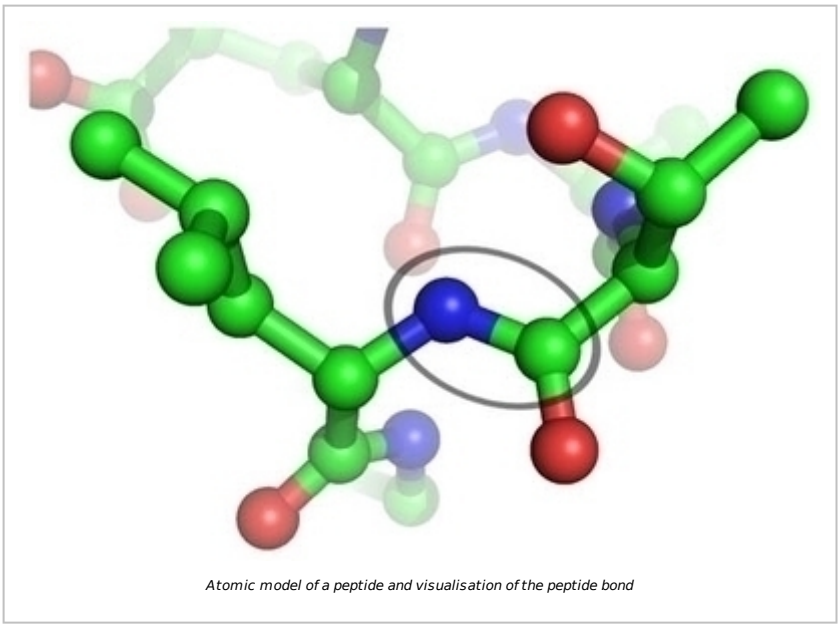
KEYWORD(S) : Protein / Molecular Dynamics / Heat Transfer

SCIENTIFIC CONTEXT :

Proteins are molecular machines that need to transport energy to work and function. Two phenomena support this heat transfer: Propagation of conformational changes and removal of excess heat. To describe this second mechanism, the heat flow can be detected via time-resolved vibrational spectroscopy [1]. Another approach to investigate heat transfer is to run non-equilibrium molecular dynamics (MD) simulations, depositing energy into one vibrational mode and following its flow through the protein directly as a function of time.



Atomic model of a peptide and visualisation of the peptide bond

MISSIONS :

After a bibliographical review, the student will perform classical molecular dynamics simulation of peptides in water using existing, standard molecular dynamics packages (openMM or LAMMPS). The system will be build using all-atom models and the simulations run on the ILM computing facility using linux operating systems. The trajectories obtained are going to be analyzed in terms of heat transfer using python scripts. In particular, we are interested in the impact of the protein structure on the dynamics of removal of excess heat towards the solvent. Simulations starting with different secondary structures (helices or sheets) are going to be compared. Interest for programming, biophysics or soft matter are important.

OUTLOOKS :

The student will acquire knowledge on molecular simulation tools, and on biomolecules.

BIBLIOGRAPHY :

[1] Botan, V., Backus, E. H. G., Pfister, R., Moretto, A., Crisma, M., Toniolo, C., Nguyen, P. H., Stock, G., & Hamm, P. (2007). Energy transport in peptide helices. www.pnas.org/cgi/content/full/

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