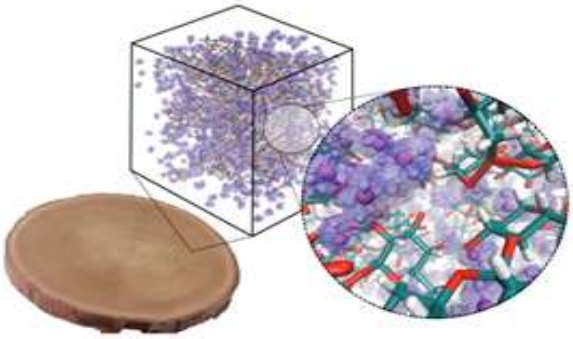
# Molecular Dynamics Approach to Water Sorption Phenomena in Wood

Romain Dupuis & Bruno Clair

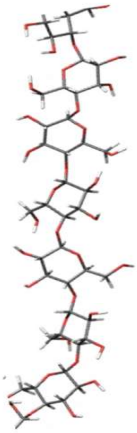
Laboratory of mechanics and civil engineering

**Wood is a bio-sourced material with a low energy cost of production. It can be produced locally, is renewable, and biodegradable. Additionally, wood is the primary terrestrial carbon stock, and its use extends carbon storage beyond the life of the tree.**

Wood is a cellular material with walls composed of a cellulose fiber composite in a matrix of hemicellulose and lignin. These walls are highly hydrophilic, and variations in air humidity will alter the water content of the walls, thereby affecting the dimensions and physical and mechanical characteristics of the wood. Understanding the role of water during drying and hydration cycles is crucial for numerous applications, particularly in construction and the conservation of wooden heritage objects.

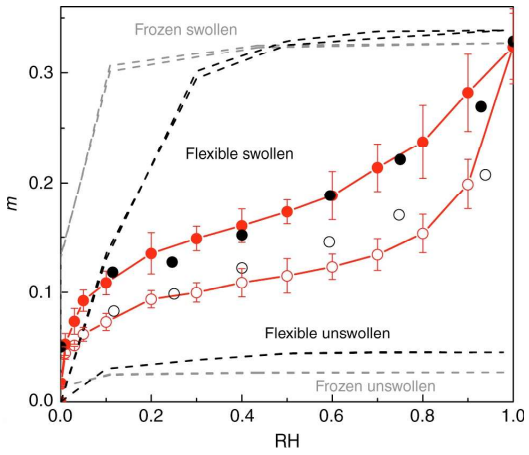


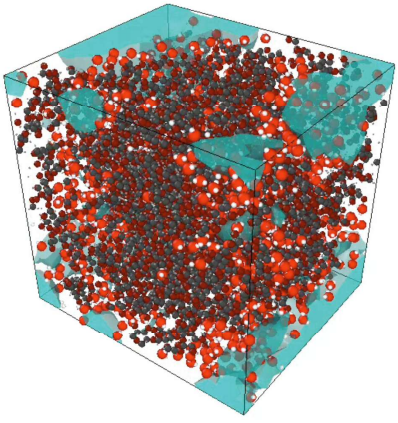
In recent years, molecular simulations have been increasingly used to study the behavior of water in cellulose models[1]. However, the impact of wood composition, particularly the amounts of cellulose, lignin, and hemicellulose, on water dynamics and adsorption has not been fully explored. This project aims to simulate the water adsorption-desorption isotherm in wood using model systems to better understand the interaction between water and pores. One objective is to understand more precisely the origin of hysteresis that is observed experimentally on the adsorption-desorption curves.



**cellulose fiber**

**adsorption isotherm**



Example simulation of water sorption in cellulose performed by Haleh Ghanei (LMGC, Montpellier)

[1] Chen et al. "Wood–Moisture Relationships Studied with Molecular Simulations: Methodological Guidelines" Forests 2019