Ph.D. defense

Institut de Chimie Séparative de Marcoule / CEA Marcoule
(UMR 5257, CEA, CNRS, Université Montpellier, ENSCM)

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will present his Ph.D. dissertation

Thermodynamics of water adsorption in model structured molecular systems including analogues of hemicelluloses, crystalline cellulose and lignin

The defense will take place on **Monday, November 20, 2017** at **2.30 pm**

in the ICSM Auditorium

The so-called “wood material” is a complex, highly anisotropic and hierarchically organized nanocomposite. At the nanometric scale, it is characterised by stiff crystalline cellulose nanofibres parallel to each others embedded in a matrix of a much softer, less anisotropic, gel of hemicelluloses, lignin and water. This matrix is hygroscopic and the solvent uptake is controlled by molecular forces like entropy, H-bonding of polysaccharides to cellulose nano-crystals and hydration force. The swelling provides a source of internal stress for the cellulose fibrils that, winding with a spiral angle (the microfibril angle, MFA) around the central lumen, passively reorient following the osmotic stress applied to them. Depending on the MFA, wood fibres exhibit a wide range of behaviors and mechanical properties, being able to act as stiff material to bear load, or shrink or expand in the longitudinal direction upon swelling, generating in this way either large tensile or compressive stresses or large strains.

For the first time, the equation of state including entropic, chemical, colloidal terms (as the hydration force) as well as the mechanical, macroscopic, term has been established and allows to predict with a parameterless analytical expression, the water absorption of untreated softwoods as a function of relative humidity changes.

The aim of the thesis is to extend this first equation of state to describe wood treatments by electrolytes adsorption in hydrothermal conditions. The experimental part is performed using specific sorption devices as well as X-Ray scattering techniques. The theoretical part is developed extending the established master equation linking molecular level chemical forces, colloidal interactions and mechanics. The results of the model are tested against experimental data of electrolytes adsorption and compared with their chaotropic/cosmotropic character according to the Hofmeister series.

Nowadays, several wood treatments have been developed to reduce the water uptake by wood, in order to confer higher resistance to moist to low-quality wood materials. The final aim of the project is to test the prediction of the model against these known treatments and to develop a general model to describe the behaviour of the wood under different chemical and physical environments. This way, new treatments can be conceptually designed and pre-existing treatments (as for instance the patented “woodprotect” one) improved.

Keywords: Thermodynamics; water; adsorption; hemicelluloses; cellulose; lignin