



"Soft-Matter Seminar"

Dr. Jean-Francois Dufreche

University P. et M. Curie, Paris, France

Title:

Dynamics of ions in electrolyte solutions: from bulk solutions to confined media

Abstract:

Since the pioneering works of Debye, Huckel and Onsager, equilibrium and transport properties of ions in electrolyte solutions are understood in terms of continuous solvent models for which the molecular nature of the solvent is neglected. However this simplified description is not enough for the general case, and general coarse-graining procedures which treat the solvent effects more precisely have to be carried out. We will present such approaches in the case of electrolyte solutions. For bulk solutions, we will show how a multiscale approach can describe the dynamics of nanoparticles from Brownian dynamics simulations. The case of ions confined in clays will also be presented. For hydrated montmorillonite clays, the Donnan effect (i.e salt exclusion in a confined system) will be described from a multi-scale procedure. For dehydrated clays with very low water contents, we will show how it is in fact possible to derive continuous solvent models for the dynamics of heavy ions. Such a description is particularly important for the storage of nuclear wastes which is controlled by the diffusion of heavy elements in a clay barrier.

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16:00 Uhr
Raum PH 3344

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