ESPCI
Laboratoire PMMH
10 rue Vauquelin, 75231 Paris Cedex 05

Séminaire PMMH

Bureau d'Études, Bâtiment L, 2 ème étage

Vendredi 18 novembre 2016, 11h00-12h00

Maximilien Levesque

laboratoire PASTEUR, Ecole Normale Supérieure

The one molecule in a sea of others : tackling solvation at the molecular scale

Physical and chemical processes in the liquid and gas phases happen in an embedding medium, a large number of solvent molecules, for instance water, that crowd the environment. To take into account this environment at the molecular scale, several possibilities are offered to in-silico experimentalists :
(i) One can forget about the molecular nature of the solvent : no hydrogen bonding, no crowding effect, etc. These primitive methods focus on macroscopic properties of the solvent like its dielectric permittivity : that's quite crude, but fast and arbitrarily configurable.
(ii) Very precisely, from all-atom simulations like molecular dynamics. Increase the numerical cost by 4 orders of magnitude with respect to solution (i) and you have all the details you want ; If it fits in nowadays computers.
(iii) We will discuss a new paradigm, the molecular density functional theory, and the associated code (MDFT) and startup (FAST). For the same numerical cost as primitive models, our implicit-explicit theory aims at producing, rigorously, the equilibrium properties of all-atom simulations.