Simulation of systems under thermodynamic gradients

Tuesday 25

10:00 Registration

10:45 Welcome

11:00 Roland Pellenq *Transport properties of alkanes in shale-rocks from the bottom-up approach*

11:30 Francois-Xavier Coudert *Theoretical insight into Soft Porous Crystals: Problems and tools to solve them*

12:00 Jean Francois Dufrêche *Multi-scale modeling of porous media for separation chemistry*

12:30 Amaël Obliger *Pore network model of electrokinetic transport through charged porous media*

13:00-14:30 Lunch @ L'Ardoise (on Jussieu Campus)

14:30 Ignacio Pagonabarraga *Emergent patterns in suspensions of self-phoretic colloids*

15:00 Giovanni Ciccotti *Dynamical non-equilibrium Molecular Dynamics Approach to convection*

15:30 Jure Dobnikar *Stimulus-sensitive colloidal walkers*

16:00-16:30 Coffee Break

16:30 Alessandro Siria *Nanofluidics to channel the osmotic energy*

17:00 Laurent Joly *Nanofluidic Osmotic Diodes: Theory and Molecular Dynamics Simulations*

17:30 Discussion

Wednesday 26

09:30 Alois Wurger *Charges in a temperature gradient: Thermo-electro-osmosis and related effects*

10:00 Signe Kjelstrup *The heat of transfer – an underestimated quantity*

10:30-11:00 Coffee Break

11:00 Guillaume Galliero *From thermodiffusion to thermogravitation, a molecular simulation perspective*

11:30 Fernando Bresme *Manipulating water and aqueous solutions with thermal gradients*

12:00 Marisol Ripoll *Implementation of temperature gradients in mesoscopic simulations*

12:30-14:00 Lunch @ L'Ardoise (on Jussieu Campus)

14:00-14:30 Carlos Nieto-Draghi *NEMD simulation techniques applied to CO_2 capture and transport*

14:30-15:00 Samy Merabia *On the importance of thermal boundary resistance in nanoscale heat transfer*

15:00-15:30 Bernard Rousseau *Thermal Diffusion in simple fluid mixtures. What have we learnt from (NE) molecular dynamics simulations?*