School on Atomistic Simulation Techniques

23 - 24 September, 2013

Monday 23/09

9:30-10:30	**Introduction to DFT and solid state physics concepts I** *Geoffrey Pourtois*
10:30-11:00	Coffee break
11:00-12:00	**Introduction to DFT and solid state physics concepts II** *Geoffrey Pourtois*
12:00-13:00	**Dispersion in DFT** *Alisa Krishtal*
13:00-14:00	Lunch
14:00-15:00	**Basics of molecular dynamics and Monte Carlo simulations I** *Barend Thijsse*
15:00-15:30	Coffee break
15:30-16:30	**Basics of molecular dynamics and Monte Carlo simulations II** *Barend Thijsse*
16:30-17:30	**Monte Carlo simulations: canonical vs. grand canonical ensemble** *Hakim Amara*

Tuesday 24/09

	First principle chemical kinetics of reactions in gas phase, solution and nanoporous materials *Veronique van Speybroeck*
	Coffee break
	Dielectric, vibrational and thermodynamic properties of solids *Xavier Gonze*
	Tight-binding formalism: from electronic structure to energetics *Hakim Amara*
	Lunch
	Phenomenological models for the thermodynamics and kinetics in nano-systems *Nele Moelans*
	Coffee break
	Free energy methods and multiscale modeling *James Elliott*
	Tight-binding simulations of carbon systems: GPU computations *Lucian Covaci*

Venue

University of Antwerp

Klooster van de Grauwzusters
Lange Sint-Annastraat 7, Antwerp

Organization

Organizer: Erik Neyts, UA

Participation is free, but registration is required by email to erik.neyts@uantwerpen.be

Organized in the framework of the FWO-WOG 'Computational Modeling of Materials'