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Institut Català d'Investigació Química

2013 Seminar Program

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Av. Països Catalans, 16, Campus Sescelades (St. Pere i St. Pau), Tarragona. Tel. 977920200

Towards an Atomistic Picture of The Active Interface in Dye Sensitized Solar Cells

Prof. Dr. Joost VandeVondele

Nanoscale Simulations, ETH Zurich (Switzerland)

Friday 26th April, 2013. ICIQ Auditorium, 12 p.m.

Professional career

Nov 2011 – present: Assistant Professor Nanoscale Simulation, ERC starting grant: development of modeling tools for the nanoscale, solar cells. ETH Zurich, Switzerland

Nov 2005 - Oct 2011: Oberassistent: Dye sensitized solar cells, radicals in solution, massively parallel DFT, large scale atomistic simulations, new methods for Hartree-Fock exchange. University of Zurich, Switzerland c/o Prof. J. Hutter

Jan 2003 - Oct 2005: Marie Curie Fellow: Early steps in radiation damage, electron transfer reactions and radicals, ab initio simulation of liquids. University of Cambridge, UK c/o Prof. M. Sprik

Jan 2002 - Nov 2002: Postdoctoral researcher: Linear scaling DFT and efficient ab initio molecular dynamics for large systems. CP2K/Quickstep development. University of Zurich, Switzerland c/o Prof. J. Hutter

Oct 1998 - Dec 2001: Ph.D. student (awarded the ETH medal): Extending length and time scales of ab initio molecular dynamics, QM/MM simulations and enhanced sampling. CPMD development. ETH Zurich, Switzerland c/o Prof. U. Rothlisberger

Oct 1993 - Jul 1998: Engineering with specialisation in physics. University of Ghent, Belgium

Research Interests

The research focus is on the development of new methods to enable ab initio molecular dynamics simulations of complex systems with modern density functional theory. New methods, implemented for massively parallel computers, are applied to a wide range of systems such as radicals in clusters and the condensed phase, surface physics, and interfacial systems such as dye sensitized solar cells.