

**Programme of the ITN-ARGENT mini-workshop
May 4-5, 2016**

**Venue: Otto-Stern-Zentrum, Seminar Room 4
Campus Riedberg, Goethe University (GU)
Ruth-Moufang-Str. 2, Frankfurt am Main**

**Organisers: Nigel Mason (OU), Stefan Schramm (GU),
Andrey Solov'yov (MBN RC)**

Wednesday, May 04, 2016

- **9.30 - 10.15.** Andrey V. Solov'yov (MBN-RC, Frankfurt am Main, Germany):
Opening address. Multiscale modelling of radiation driven processes in complex molecular systems.
- **10.15 - 11.00.** Kurt Stokbro (QuantumWise, Copenhagen, Denmark):
Atomic-scale modelling using the Atomistix ToolKit from QuantumWise.
- **11.00 - 11.30.** Coffee break.
- **11.30 - 12.15.** Mai Dinh (UPS, Toulouse, France):
Core-excited resonances in electron attachment on water: from mean-field calculations and beyond.
- **12.15 - 13.00.** Kaspar Haume (OU, Milton Keynes, UK):
Molecular dynamics simulations of PEG coated gold nanoparticles for medical applications.
- **13.00 - 14.30.** Lunch.
- **14.30 - 15.15.** Eugene Surdutovich (OU, Oakland, USA):
Transport of secondary particles and the onset of shock waves in ion's tracks.
- **15.15 - 16.00** Herbert M. Urbassek (UK, Kaiserslautern, Germany)
Effect of swift-ion irradiation on DNA molecules: a molecular dynamics study using the REAX force field.
- **16.00 - 16.30.** Coffee break.
- **16.30 - 17.15.** Pablo de Vera (QUB, Belfast, UK):
Studying ion-induced thermomechanical DNA damage by atomistic simulations.
- **17.15 - 18.00.** Alexey Verkhovtsev (CSIC, Madrid, Spain):
Multiscale approach predictions for biological outcomes in ion-beam cancer therapy.

19.00 Conference dinner.

Thursday, May 5, 2016.

- **9.00 - 9.45.** Nigel Mason (OU, Milton Keynes, UK):
Modelling electron interactions with molecular species.
- **9.45 - 10.30.** Gustavo Garcia (CSIC, Madrid, Spain)
Low energy secondary particle track simulation in positron beam irradiation of water.
- **10.30 - 11.15.** Balder Villagomez-Bernabe (QUB, Belfast, UK):
Overview of the work carried out in the Nano-scale Radiation Physics group at QUB.
- **11.15 - 11.45.** Coffee break.
- **11.45 - 12.30.** Chris Kexel (MBN RC, Frankfurt am Main, Germany):
Surface chemistry of thin films studied with MBN Explorer.
- **12.30 - 13.15.** Christof Verlackt (University of Antwerp, Belgium):
Multi-level modeling approach for plasma medicine.
- **13.15 - 15.00.** Lunch and Departure.