

The First Quantemol Workshop

"Linking Simulation and Experiment"

Date: 10th June 2011

Place: University College London, Physics and Astronomy Department

Speakers:

- **Prof. Nick Braithwaite** (Professor of Engineering and head of the department of Physics and Astronomy at the Open University. Research is in plasma physics, studies of plasmas formed from electrical discharges in gasses as part of technological applications relating to the manufacture of semi-conductors)

- **Prof. Nigel Mason** (Professor of Molecular Physics and Director of Research in Department of Physics and Astronomy at the Open University, Order of the British Empire, leads a research group exploring many different facets of molecular physics including: astrochemistry; atmospheric physics; plasma chemistry and radiation chemistry)

- **Prof. Zoran Petrovic** (Director of Gaseous Electronics Laboratory at the Institute of the physics in Zemun, Belgrade. His research into the physics of ionized gases motivated by possible non-equilibrium plasma applications; he also studies in charged particle swarms, low pressure breakdown and discharges and kinetics and applications of collisional plasmas.)

- **Prof. Jonathan Tennyson** (Professor of Physics, Fellow of The Royal Society, Head of Department of Physics and Astronomy at the University College London. Maintains and develops R-matrix codes for modelling the low energy scattering of electrons and positrons by molecular targets)

- **Prof. Leanne Pitchford** (Research director at CNRS, at the " Laboratoire des Plasmas et Conversion d'Energie ", Université Toulouse. Among her research works is simulating the transport of charged particles in cold plasmas, and on simulating the plasma/electrode interaction)

The program

10:00 – 11:00

Registration, coffee and tea
Room E7, ground floor, Physics Building

11:00 – 12:55

Session 1: Modelling Plasma & Simulations presentations, Chair Anna Dzarasova
Room E7, ground floor, Physics Building

11:00 – 11:20

“Latest developments in R-matrix Theory” J. Tennyson, FRS

11:25 – 11:35

“LX Cat - an open-access web resource of data required for modeling low temperature plasmas” L. Pitchford

11:40 – 12:00

“2D Modelling of Transient Phenomena in Plasmas”, N. St. J. Braithwaite and M. Bowden

12:05 – 12:25

“Why are swarm studies important as a bridge between atomic and molecular collision data and plasma modeling” Z. Petrovic

12:30 – 12:50

“Electron induced chemistry – applications from Astrochemistry to cancer therapy”, N. J. Mason, OBE

12:55 – 13:40

Buffet lunch
Room E1, ground floor, Physics Building

13:40 – 15:45

Session 2: Simulation discovery session, two parallel hands on sessions (Quantemol-N and Quantemol-D)
Room A19, third floor, Physics Building

13:40 – 14:15

Quantemol software tutorial session

14:15 – 14:45

Coffee break
Room A17, third floor, Physics Building

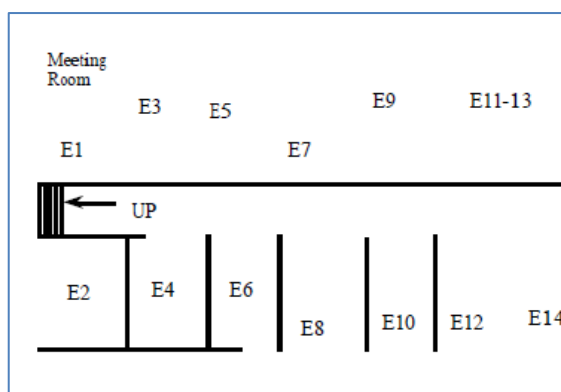
14:45 – 15:45

Quantemol-D and Quantemol-N parallel hands on sessions

15:45 – 17:00

Drinks reception
Room A13, third floor, Physics Building

Location of rooms E7 and E1, Ground floor



Location of rooms A13 and A19, Third floor

