

Warwick EPSRC Symposium 2008/2009
Challenges in Scientific Computing
 Organiser: Andrew Stuart

Workshop on Quantum Simulations

Monday 24th – Friday 28th August 2009

Organiser: R. Römer (Physics) and A. Troisi (Chemistry)

Programme

All talks will be in Lecture Room B3.02 • Mathematics Institute • Zeeman Building

Monday, August 24th, 2009

- 09:30-11:00 **Registration** in the MRC Room B1.37 and Coffee in the Common Room
 11:00-11:15 **Welcome**
 11:15-11:45 **David Logan** (Oxford) *Electron transport in multilevel quantum dots*
 11:50-12:25 **Roderick MacKenzie** (London) *A numerical study of mobility in thin films of fullerene derivatives*
 12:25-14:30 Lunch in the Mathematics Institute Common Room
 14:30-15:00 **Spiros Skourtis** (Cyprus) *Biological and small molecule electron transfer processes: some interesting connections*
 15:05-15:35 **Pablo Serna** (Murcia) *Conductivity in random resistor networks*
 15:40-16:15 Tea Break
 16:15-16:45 **Gilberto Teobaldi** (London) *The role of interstitial Ti atoms and O vacancy sites in the Ti(3d) defect states in the band gap of Titania*
 16:50-17:20 **Francisco Dominguez-Adame** (Madrid) *Polarons in DNA at finite temperature*
 17:25-18:00 Wine and cheese in the Mathematics Institute Common Room

Tuesday, August 25th, 2009

- 09:00-09:30 **Yi Luo** (Stockholm) *Dynamics and statistics of electron transport in single molecules*
 09:35-10:05 **Colin Lambert** (Lancaster) *Controlled electron transport through single molecules*
 10:10-10:40 **Vladimir Dobrosavljevic** (NHMFL Florida) *Infinite randomness fixed point of the disordered Mott transition?*
 10:45-11:15 Coffee Break
 11:15-11:45 **Peter van Dongen** (Mainz) *Doped asymmetric two-band Hubbard models*
 11:50-12:20 **Alberto Rodriguez-Gonzalez** (Warwick) *Multifractal analysis with the probability density function at the three-dimensional Anderson transition*
 12:25-14:30 Lunch in the Mathematics Institute Common Room
 14:30-15:00 **Stefano Corni** (Modena) *Modelling protein-surface interactions: a challenge for computations*
 15:05-15:35 **Eduardo Miranda** (Campinas) *The disordered Mott metal-insulator transition*
 15:40-16:15 Tea Break
 16:15-16:45 **Theodoros Papadopoulos** (Bath) *Exciton migration in conjugated polymers: the influence of positional and energetic disorder*
 16:50-17:25 **Michael Schreiber** (Chemnitz) *The modified sharpened index h_{ms} and other variants in the Hirsch index zoo*
 17:25-18:00 Wine and cheese in the Mathematics Institute Common Room

Wednesday, August 26th, 2009

- 09:00-09:30 **Antonio Rodriguez** (Madrid) *Introduction to nonextensive statistical mechanics*
 09:35-10:05 **Guioamar Ruiz-Lopez** (Madrid) *Applications of nonextensive statistical mechanics to a new universality class of unimodal dissipative maps*
 10:10-10:40 **Ulrich Kleinekathöfer** (Bremen) *Optical control of transport through molecular junctions*
 10:45-11:15 Coffee Break
 11:15-11:45 **Volkhard May** (Berlin) *Mixed quantum-classical description of electronic excitation energy transfer in supramolecular complexes*
 11:50-12:20 **Felix Hanke** (Liverpool) *Ab initio atomistic thermodynamics of oxygen adsorption in graphene vacancies*
 12:25-14:00 Lunch in the Mathematics Institute Common Room
 14:30 **Conference Excursion and River Cruise+Dinner**
 22:45 **Returning**

Thursday, August 27th, 2009

- 09:00-09:30 **Keith Slevin** (Osaka) *Critical exponent for the quantum Hall transition*
 09:35-10:05 **Oleg Prezhdo** (Seattle) *Dynamics on the nanoscale: Time-domain ab initio studies of quantum dots and carbon nanotubes*
 10:10-10:40 **Michael Schreiber** (Chemnitz) *Quasicrystals - disordered insulating metals with five-fold symmetry*
 10:45-11:15 Coffee Break
 11:15-11:45 **Simone Fratini** (Grenoble) *Band-like motion and incoherent diffusion in organic molecular semiconductors: two sides of the same coin*
 11:50-12:20 **Karsten Hannewald** (Jena) *Polaron transport in organic semiconductors: theory and modelling*
 12:25-14:40 Lunch in the Mathematics Institute Common Room
 14:30-15:00 **Josef Oswald** (Leoben) *A non-equilibrium network model for magneto transport in the quantum Hall effect regime*
 15:05-15:35 **Tapash Chakraborty** (Winnipeg) *DNA magnetism: A new paradigm in nano-bio-electronics*
 15:40-16:15 Tea Break
 16:15-16:45 **David Cheung** (Warwick) *Bottom-up modelling of charge transport in soft materials*
 16:50-17:20 **Alessandro Pecchia** (Rome) *Electron-vibration scattering in molecular transport*
 17:25-18:00 Wine and cheese in the Mathematics Institute Common Room

Friday, August 28th, 2009

- 09:00-09:30 **Sri Chaitanya Das Pemmaraju** (Dublin) *Non-equilibrium electron transport in dry DNA*
 09:35-10:05 **Manuel Pino-Garcia** (Madrid) TBA
 10:10-10:40 **David Beljonne** (Mons) *Beyond Förster resonance energy transfer in biological and nanoscale systems*
 10:45-11:15 Coffee Break
 11:15-11:45 **Stephen A. Wells** (Warwick) *Rigid proteins and conducting DNA*
 11:50-12:20 **Jose A. Hoyos** (Duke) *Edge states of quantum antiferromagnets*
 12:25-14:30 Lunch in the Mathematics Institute Common Room



If you have any questions during the workshop please see either Hazel Higgins or Yvonne Collins in Room B1.37 opposite the Common Room