**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

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
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</thead>
<tbody>
<tr>
<td>09:30-11:00</td>
<td>Registration in the MRC Room B1.37 and Coffee in the Common Room</td>
</tr>
<tr>
<td>11:00-11:15</td>
<td>Welcome</td>
</tr>
<tr>
<td>11:15-11:45</td>
<td>David Logan (Oxford) Electron transport in multilevel quantum dots</td>
</tr>
<tr>
<td>12:25-14:30</td>
<td>Lunch in the Mathematics Institute Common Room</td>
</tr>
<tr>
<td>14:30-15:00</td>
<td>Spiros Skourtis (Cyprus) Biological and small molecule electron transfer processes: some interesting connections</td>
</tr>
<tr>
<td>15:05-15:35</td>
<td>Pablo Serna (Murcia) Conductivity in random resistor networks</td>
</tr>
<tr>
<td>15:40-16:15</td>
<td>Tea Break</td>
</tr>
<tr>
<td>16:15-16:45</td>
<td>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</td>
</tr>
<tr>
<td>16:50-17:20</td>
<td>Francisco Dominguez-Adame (Madrid) Polarons in DNA at finite temperature</td>
</tr>
<tr>
<td>17:25-18:00</td>
<td>Wine and cheese in the Mathematics Institute Common Room</td>
</tr>
</tbody>
</table>

### Tuesday, August 25th, 2009

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
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</thead>
<tbody>
<tr>
<td>09:00-09:30</td>
<td>Yi Luo (Stockholm) Dynamics and statistics of electron transport in single molecules</td>
</tr>
<tr>
<td>09:35-10:05</td>
<td>Colin Lambert (Lancaster) Controlled electron transport through single molecules</td>
</tr>
<tr>
<td>10:10-10:40</td>
<td>Vladimir Dobrosavljevic (NHMFL Florida) Infinite randomness fixed point of the disordered Mott transition?</td>
</tr>
<tr>
<td>10:45-11:15</td>
<td>Tea Break</td>
</tr>
<tr>
<td>11:15-11:45</td>
<td>Peter van Dongen (Mainz) Doped asymmetric two-band Hubbard models</td>
</tr>
<tr>
<td>11:50-12:20</td>
<td>Alberto Rodriguez-Gonzalez (Warwick) Multifractal analysis with the probability density function at the three-dimensional Anderson transition</td>
</tr>
<tr>
<td>12:25-14:30</td>
<td>Lunch in the Mathematics Institute Common Room</td>
</tr>
<tr>
<td>14:30-15:00</td>
<td>Stefano Corni (Modena) Modelling protein-surface interactions: a challenge for computations</td>
</tr>
<tr>
<td>15:05-15:35</td>
<td>Eduardo Miranda (Campinas) The disordered Mott metal-insulator transition</td>
</tr>
<tr>
<td>15:40-16:15</td>
<td>Tea Break</td>
</tr>
<tr>
<td>16:15-16:45</td>
<td>Theodoros Papadopoulos (Bath) Exciton migration in conjugated polymers: the influence of positional and energetic disorder</td>
</tr>
<tr>
<td>16:50-17:25</td>
<td>Michael Schreiber (Chemnitz) The modified sharpened index h_{ms} and other variants in the Hirsch index zoo</td>
</tr>
<tr>
<td>17:25-18:00</td>
<td>Wine and cheese in the Mathematics Institute Common Room</td>
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### Wednesday, August 26th, 2009

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
</tr>
</thead>
<tbody>
<tr>
<td>09:00-09:30</td>
<td>Antonio Rodriguez (Madrid) Introduction to nonextensive statistical mechanics</td>
</tr>
<tr>
<td>09:35-10:05</td>
<td>Guiomar Ruiz-Lopez (Madrid) Applications of nonextensive statistical mechanics to a new universality class of unimodal dissipative maps</td>
</tr>
<tr>
<td>10:10-10:40</td>
<td>Ulrich Kleinekathöfer (Bremen) Optical control of transport through molecular junctions</td>
</tr>
<tr>
<td>10:45-11:15</td>
<td>Coffee Break</td>
</tr>
<tr>
<td>11:15-11:45</td>
<td>Volkhard May (Berlin) Mixed quantum-classical description of electronic excitation energy transfer in supramolecular complexes</td>
</tr>
<tr>
<td>11:50-12:20</td>
<td>Felix Hanke (Liverpool) Ab initio atomistic thermodynamics of oxygen adsorption in graphene vacancies</td>
</tr>
<tr>
<td>12:25-14:00</td>
<td>Lunch in the Mathematics Institute Common Room</td>
</tr>
<tr>
<td>14:30</td>
<td>Conference Excursion and River Cruise+Dinner</td>
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<tr>
<td>22:45</td>
<td>Returning</td>
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</tbody>
</table>
### Thursday, August 27th, 2009

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
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<tbody>
<tr>
<td>09:00-09:30</td>
<td>Keith Slevin (Osaka)</td>
<td>Critical exponent for the quantum Hall transition</td>
</tr>
<tr>
<td>09:35-10:05</td>
<td>Oleg Prezdo (Seattle)</td>
<td>Dynamics on the nanoscale: Time-domain ab initio studies of quantum dots and carbon nanotubes</td>
</tr>
<tr>
<td>10:10-10:40</td>
<td>Michael Schreiber (Chemnitz)</td>
<td>Quasicrystals - disordered insulating metals with five-fold symmetry</td>
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<tr>
<td>10:45-11:15</td>
<td>Coffee Break</td>
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<tr>
<td>11:15-11:45</td>
<td>Simone Fratini (Grenoble)</td>
<td>Band-like motion and incoherent diffusion in organic molecular semiconductors: two sides of the same coin</td>
</tr>
<tr>
<td>11:50-12:20</td>
<td>Karsten Hannewald (Jena)</td>
<td>Polaron transport in organic semiconductors: theory and modelling</td>
</tr>
<tr>
<td>12:25-14:40</td>
<td>Lunch in the Mathematics Institute Common Room</td>
<td></td>
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<tr>
<td>14:30-15:00</td>
<td>Coffee Break</td>
<td></td>
</tr>
<tr>
<td>15:05-15:35</td>
<td>Tapash Chakraborty (Winnipeg)</td>
<td>DNA magnetism: A new paradigm in nano-bio-electronics</td>
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<td>15:40-16:15</td>
<td>Tea Break</td>
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<tr>
<td>16:15-16:45</td>
<td>David Cheung (Warwick)</td>
<td>Bottom-up modelling of charge transport in soft materials</td>
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<tr>
<td>16:50-17:20</td>
<td>Alessandro Pecchia (Rome)</td>
<td>Electron-vibration scattering in molecular transport</td>
</tr>
<tr>
<td>17:25-18:00</td>
<td>Wine and cheese in the Mathematics Institute Common Room</td>
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<tbody>
<tr>
<td>09:00-09:30</td>
<td>Sri Chaitanya Das Pemmaraju (Dublin)</td>
<td>Non-equilibrium electron transport in dry DNA</td>
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<tr>
<td>09:35-10:05</td>
<td>Manuel Pino-Garcia (Madrid)</td>
<td>TBA</td>
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<tr>
<td>10:10-10:40</td>
<td>David Beljonne (Mons)</td>
<td>Beyond Förster resonance energy transfer in biological and nanoscale systems</td>
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<td>10:45-11:15</td>
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<td>11:15-11:45</td>
<td>Stephen A. Wells (Warwick)</td>
<td>Rigid proteins and conducting DNA</td>
</tr>
<tr>
<td>11:50-12:20</td>
<td>Jose A. Hoyos (Duke)</td>
<td>Edge states of quantum antiferromagnets</td>
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If you have any questions during the workshop please see either Hazel Higgens or Yvonne Collins in Room B1.37 opposite the Common Room