Euro-TMCS II Theory, Modelling & Computational Methods for Semiconductors
7th December 2016 to 9th December 2016
Location: Cork, Ireland


10:30-11:30  Registration (A.6.G.34)

11:30-12:20  Matt Probert (University of York) Plane-Wave DFT and LDA

12:20-13:10  Ben Hourahine (University of Strathclyde) DFT-Tight-Binding Theory

13:10-14:15  Lunch (B.0.17)

14:15-15:05  Stefano Sanvito (Trinity College Dublin) Non-equilibrium Green’s Function Methods

15:05-15:55  Fabio Sacconi (TiberLAB) Device Simulations

15:55-16:25  Coffee Break

16:25-17:15  Jacky Even (CNRS) Modelling of Halide Perovskites

**Day 2: 8th December 2016: University College Cork (Aula Maxima & Devere Hall)**

08:30-09:00  Registration (outside Aula Maxima)

09:00-09:15  Welcome (Aula Maxima)

**Session 1:** 2-D Materials (Aula Maxima)
        Session Chair: Stanko Tomic (University of Salford)

09:15-09:45  Thierry Amand (INSA Toulouse) Exciton dynamics and spin-orbit effects in atomically thin TMDC and their alloys

09:45-10:00  Hsin Lin (National University of Singapore) Topological Materials

10:00-10:15  Mahdi Shirazi (Technical University of Eindhoven) Sulfurization of 2D material: a multi-scale modelling study

10:15-10:30  Miša Andelković (University of Antwerp) Large-scale conductivity calculations of (twisted) bilayer graphene

10:30-10:45  Samuel Magorrian (University of Manchester) Electronic and optical properties of two-dimensional InSe from DFT-parameterised tight-binding model

10:45-11:15  Coffee Break
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<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
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<td>11:15-11:30</td>
<td>Ludwig A. Th. Grief</td>
<td>Modeling Energy Transfer Processes in GaN Quantum Wires</td>
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<td>11:30-11:45</td>
<td>Oliver Marquardt</td>
<td>Influence of strain relaxation in axial In\textsubscript{x}Ga\textsubscript{1-x}N/GaN nanowire heterostructures on their electronic properties</td>
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<td>11:45-12:00</td>
<td>Ramzi Benchamekh</td>
<td>Impact of random alloy fluctuations on the electronic and optical properties of site-controlled (111)-oriented InGaAs/GaAs quantum dots</td>
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<td>12:00-12:15</td>
<td>Daniel Tanner</td>
<td>Elastic properties of semiconductors beyond the limit of infinitesimal strain</td>
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<td>12:15-12:30</td>
<td>Elena Pascal</td>
<td>Theoretical model of threading dislocations strain and contrast in the scanning electron microscope images</td>
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<td>12:30-13:00</td>
<td>Poster Presentations: 2 minute Poster Presentations</td>
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PO13. **Luke Wilson** (Swansea University) Study of the impact of electrodes in the electron transport through Guanine and 8-oxoGuanine

PO14. **Ben Hourahine** (University of Strathclyde) Semi-emperical time-dependent DFT for plasmonic systems

PO15. **Orest Malyk** (Lviv Polytechnic National University) The local electron interaction with crystal lattice defects in cadmium telluride: ab initio approach

13:00-14:45 Lunch & Poster Session (*Devere Hall*)

**Session 3:** DFT + Fundamentals (*Aula Maxima*)
Session Chair: **Matt Probert** (University of York)

14:45-15:15 **Patrick Rinke** (Aalto University) Charge transfer at organic-inorganic interfaces

15:15-15:30 **Manveer Singh Munde** (University College London) Mechanism for Oxygen Vacancy Accumulation Under Electron Injection Conditions in Amorphous Silicon Oxides

15:30-15:45 **Miguel A. Caro** (Aalto University) Amorphous carbon as a versatile semiconductor material for analytical electrochemistry

15:45-16:00 **Ben Hourahine** (University of Strathclyde) Making Correlated Systems More Tractable

16:00-16:30 Coffee Break

**Session 4:** New Materials (*Aula Maxima*)
Session Chair: **Patrick Rinke** (Aalto University)

16:30-17:00 **Ivana Savic** (Tyndall National Institute) Modelling of the thermoelectric properties of materials near soft mode phase transitions

17:00-17:15 **Mikael Råsander** (Imperial College London) Physical properties of the wide band gap II-IV nitride MgSiN₂

17:15-17:30 **Laurentiu Baschir** (National Institute R&D of Optoelectronics) Surface plasmon resonance simulations in structures with chalcogenide layer

17:30-17:45 **William Armando Munoz** (Linköping University) On the insulator to semimetallic transition in conducting polymers

17:45-18:00 **Frank C. Maier** (University of Stuttgart) DNA sequencing using diamondoid-functionalized nanopores

19:30 Networking Dinner at South’s Bar at The Imperial Hotel
**Day 3: 9th December 2016: University College Cork (Aula Maxima)**

**Session 1:** Hybrid Perovskites + Solar Cells *(Aula Maxima)*  
Session Chair: *Ivana Savic* (Tyndall National Institute)

09:00-09:30  
*Mark van Schilfgaarde* (King’s College London) Hybrid Perovskites

09:30-09:45  
*Matro Mužević* (University of J. J. Strossmayer in Osijek) Band gap engineering in perovskites as solar cell buffer layers

09:45-10:00  
*Urs Aeberhard* (Forschungszentrum Jülich) Computational challenges in the NEGF simulation of mesoscopic solar cell components

10:00-10:15  
*Slobodan Čičić* (University of Salford) Heuristic modelling of multi-junction solar cells

10:15-10:30  
*Philippe Czaja* (Forschungszentrum Jülich) Optoelectronic properties of a-Si:H and a-Si:H.c-Si interfaces from first principles

10:30-11:00  
Coffee Break

**Session 2:** Device Simulations *(Aula Maxima)*  
Session Chair: *Miguel A. Caro* (Aalto University)

11:00-11:30  
*Yuh-Renn Wu* (National Taiwan University) Challenges in Optoelectronic Device Simulation

11:30-11:45  
*Fabio Sacconi* (TiberLAB) Effects of strain distribution on the emission properties of (In,Ga)N/GaN nanowire LEDs

11:45-12:00  
*Christopher A. Broderick* (University of Bristol) Theory of InGaBiAs/InP mid-infrared semiconductor lasers

12:00-12:15  
*Antonio Martinez* (Swansea University) Impact of Short range Coulomb repulsion on the current through a 1D Nanostructure

12:15-12:30  
*Pedram Razavi* (Tyndall National Institute) Effect of alloy and dopant scattering in In$_{1-x}$Ga$_x$As nanowires

12:30-12:45  
*Markus Kantner* (Weierstrass Institute for Applied Analysis and Stochastics) Multi-scale modelling and simulation of single-photon sources on a device level