

Euro-TMCS II Theory, Modelling & Computational Methods for Semiconductors

7th December 2016 to 9th December 2016

Location: Cork, Ireland

Day 1: 7th December 2016: Tyndall National Institute (A.6.G.34 & B.0.17)

10:30-11:30	Registration (<i>A.6.G.34</i>)
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 (<i>B.0.17</i>)
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 (<i>outside Aula Maxima</i>)
09:00-09:15	Welcome (<i>Aula Maxima</i>)
Session 1:	2-D Materials (<i>Aula Maxima</i>) 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 Anđelković (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

Session 2:

Nanostructures & Poster Presentations (*Aula Maxima*)

Session Chair: **Ben Hourahine** (University of Strathclyde)

- 11:15-11:30 **Ludwig A. Th.Grief** (Technische Universität Berlin) Modeling Energy Transfer Processes in GaN Quantum Wires
- 11:30-11:45 **Oliver Marquardt** (Paul-Drude-Institut für Festkörperelektronik) Influence of strain relaxation in axial $\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ nanowire heterostructures on their electronic properties
- 11:45-12:00 **Ramzi Benchamekh** (Tyndall National Institute) Impact of random alloy fluctuations on the electronic and optical properties of site-controlled (111)-oriented InGaAs/GaAs quantum dots
- 12:00-12:15 **Daniel Tanner** (Tyndall National Institute) Elastic properties of semiconductors beyond the limit of infinitesimal strain
- 12:15-12:30 **Elena Pascal** (University of Strathclyde) Theoretical model of threading dislocations strain and contrast in the scanning electron microscope images
- 12:30-13:00 Poster Presentations: 2 minute Poster Presentations

- PO1. **Pablo Palacios** (Universidad Politécnica de Madrid) Band Alignment between Intermediate Band Material and CuAlSe_2 and ZnS
- PO2. **Joao Abreu** (Queen's University of Belfast) First principles modelling of tunnel field-effect transistors based on heterojunctions of strained Germanium/InGaAs alloy
- PO3. **Abdoulwahab Adaine** (Université de Lorraine) Multivariate numerical optimization of an InGaN-based hetero junction solar cell
- PO4. **Hela Boustanji** (Faculté des Sciences de Tunis) Effect of thermal annealing on the performance of type-II GaSb/GaAs quantum dots solar cell
- PO5. **Silviu Bogusevschi** (Tyndall National Institute) AlGaInP-based Quantum Dot LEDs as efficient red light sources
- PO6. **Saroj Kanta Patra** (Tyndall National Institute) Theoretical study of the optical properties of a-plane InGaN/GaN quantum dots
- PO7. **Oliver Marquardt** (Paul-Drude-Institut für Festkörperelektronik) Electronic properties of GaAs crystal phase nanostructures
- PO8. **Miguel A. Caro** (Aalto University) Configurational effects on the piezoelectricity of semiconductor alloys: the case of ScAlN
- PO9. **Edmond O'Halloran** (Tyndall National Institute) Direct band gaps from GeSn alloys: A hybrid functional density functional theory based analysis
- PO10. **Rikmantra Basu** (National Institute of Technology Delhi) Tunnel Injection Transistor Lasers: A Group IV Material based Analysis
- PO11. **Federico Iori** (Université Paris Sud) Engineering $\text{SrTiO}_3/\text{LaAlO}_3$ heterostructures thickness: an abinitio study
- PO12. **Stephen Rhatigan** (Tyndall National Institute) Ceria-Titania Interfaces for CO_2 and Water Activation

- 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-empirical 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 Rålander** (Imperial College London) Physical properties of the wide band gap II-IV nitride MgSiN_2

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
http://www.flynnhotels.com/Imperial_Hotel_Cork/souths-bar.html

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

Matko 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 $\text{In}_{1-x}\text{Ga}_x\text{As}$ 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