Training Day Programme

Wednesday 22nd January 2014

10:00
Matt Probert (University of York), "Ab Initio modelling of structural and electronic properties of semiconductors"

11:30
Gyaneshwar P. Srivastava (University of Exeter), "Phonons in Nanostructures"

13:00 Lunch and Hands-on Sessions

Activity: Hands-on Session
13:30-14:30 Atomistix ToolKit tutorial

14:30
Benjamin Hourahine (University of Strathclyde), "Empirical and semi-empirical quantum mechanical methods for semiconductor modelling"

16:00
Eoin O'Reilly (Tyndall National Institute), "Multiscale Simulation – from DFT to full device modelling"
Regular Programme

Thursday 23rd January 2014

08:30 - 09:25 Coffee and registration

09:25 Opening remarks (Stanko Tomic - University of Salford)

DFT I (chair: Ben Hourahine)

09:30 Invited: CECAM distinguished lecture: Linear Scaling TD-DFT
Peter Haynes (Imperial College London, UK)
10:00 Excitons in semiconductors and related materials from time dependent density functional theory
Leonardo Bernasconi (STFC RAL, UK)
10:15 Fast, stable convergence of large, first-principles semiconductor simulations
Phil Hasnip (University of York, UK)
10:30 Spin-orbit coupling and non-collinear magnetism in the CASTEP code
Daniel R. Jones (University of Oxford, UK)
10:45 DFT calculation of the electronic structure of defects in Germanium
Helen Rafferty (University of Leeds, UK)
11:00 Ab initio calculations for group IV dopants on the surface of GaAs (110)
F. J. Tilley (University of Leicester, UK)
11:15 Non-ideal interfaces: A first principles investigation of the electronic properties of the Mo/GaAs interface
Steven P. Hepplestone (University College London, UK)
11:30 Invited: Piezoelectricity, elasticity, and deformation potentials in III-Nitrides
Slawomir Lepkowski (Polish Academy of Sciences, Institute of High Pressure Physics)

QuantumWise Presentation (chair: Max Migliorato)

11:45 Atomistix ToolKit – a platform for atomic-scale simulations of nanoelectronic devices
Anders Blom (QuantumWise-Copenhagen, Denmark)

12:45 working Lunch, Networking, Hands-on Sessions and Posters

Activity: Hands-on Session
13:15-14:15 Atomistix ToolKit tutorial

Semi-empirical methods: EPM,TB,kp (chair: Max Migliorato)

14:15 Fast simulation of quantum hydrogens in semiconductors
Ben Hourahine (University of Strathclyde, UK)
14:30 Tight binding determination of the electronic structure of low dimensional chalcogenide-based superlattices
Efterpi Kalesaki (University of Luxembourg, Luxembourg)
Programme Outline

14:45 Electron-Phonon coupling in colloidal CdSe/CdS quantum dots
Steffen Westerkamp (Technical University of Berlin, Germany)

15:00 Generalised effective-mass theory of sub-surface STM: application to impurity states
Mervyn Roy (University of Leicester, UK)

15:15 Surface Passivation of Quantum Dots
Andrew Sills (University of Leeds, UK)

15:30 Analytical solutions for the nonlinear optical absorption and photoluminescence of anisotropic semiconductor materials
M.F. Pereira (Sheffield Hallam University, UK)

15:45 Lasing properties of photonic crystal microcavities with InAsSb quantum dots
José M. Llorens (Instituto de Microelectrónica de Madrid, Spain)

16:00 Coffee Break

Multi-scale Methods (chair: Mathieu Luisier)

16:30 Multi-scale modelling of the electronic structure of dilute bismide alloys
Christopher A. Broderick (Tyndall National Institute, Cork, Ireland)

16:45 Multi-Scale Simulations of Transport through an Mo/n+-GaAs Contact
Manuel Aldegunde (Swansea University, UK)

17:00 Ab initio parameterisation of the 14 band k•p Hamiltonian: III-V Study
Mark Lundie (University of Salford, UK)

17:15 Multi-scale computational framework for evaluation of the performance of molecular based flash cells
Vihar P. Georgiev (University of Glasgow, UK)

17:30 Break for Social Dinner (19:30)
Programme Outline

Friday 24th January 2014

08:30-09:00 Registration

PV (chair: Stanko Tomic)
09:00 Invited: Modelling of the high efficiency solar cells
Ned Ekins-Daukes (Imperial College London)
09:30 Invited: Hot carriers solar cells
Jean-François Guillemoles (IRDEP, UMR CNRS, France)
10:00 Theoretical studies of biexciton binding energy in CdSe/CdTe core/shell type II quantum dots
Jacek M. Miloszewski (University of Salford, UK)
10:15 Phonon lifetime calculations for Hot Carrier Solar Cells
Sana Laribi (IRDEP Institute of Research and Development on Photovoltaic Energy, France)
10:30 Coffee Break

10:45 Kesterite solar cells: from thermodynamics to device physics from first-principles
Jarvist M. Frost (University of Bath, UK)
11:00 Multibandgaps and multivalleys hybrid perovskites for photovoltaic applications
Jacky Even (Université Européenne de Bretagne, France)
11:15 Incorporating the influence of the scanning probe in rigorous simulations by fast post-processing methods
Markus Ermes (IEK5–Photovoltaik, Germany)
11:30 Invited: Electronic structure of I-III-VI2 chalcopyrite materials and their application for thin film solar cells
Clas Persson (University of Oslo, Norway)

Transport (chair: Jean-François Guillemoles)
12:00 Invited CECAM distinguished lecture: Parallelization strategies for the NEGF Equations
Mathieu Luisier (ETH Zürich)
12:30 Causal self-energies for NEGF modelling of quantum nanowires
John Barker (University of Glasgow, UK)
12:45 Fluorescence spectra of colloidal QD: impact of QD configuration and carrier dynamics
Urs Aeberhard (IEK5–Photovoltaik, Germany)
13:00 Impact of different electron-phonon scattering models on the electron transport in a quantum wire
Anna Price (Swansea University, UK)

13:15 working Lunch, Networking, Hands-on Sessions and Posters

Graphene (chair: Christopher Castleton)
14:15 Semi-empirical phonon calculations for graphene on different substrates
Henrique Miranda (University of Luxembourg, Luxembourg)
14:30 From Diamond to Graphene: atomistic modelling of elasticity and phonons
Umberto Monteverde (University of Manchester, UK)
Programme Outline

14:45 Analysis of energy gap opening in functionalised graphene oxide
Mark Lundie (University of Salford, UK)
15:00 Electron irradiation effects on nanomechnical properties of graphene: Molecular dynamics study
Kazuhiro Tada (Toyama National College of Technology, Japan)
15:15 Optical and vibrational properties of layered MoS$_2$
Alejandro Molina-Sánchez (University of Luxembourg, Luxembourg)

15:30 Coffee Break

DFT 2 (chair: Matt Probert)
16:00 DFT studies of polaron dynamics in ceria
Christopher Castleton (University of Nottingham, UK)
16:15 Modelling electron excitation in BiVO$_4$ photoelectrodes for solar water-splitting
Rachel Crespo-Otero (University of Bath, UK)
16:30 Step Defects on the TiO$_2$ Rutile (110) Surface: A New Methodology to Get One Step Ahead of Steps
Trevor P. Hardcastle (University of Leeds, UK)
16:45 Non linear Piezoelectricity in Nanostructures and Devices
Hanan Al-Zahrani (University of Manchester, UK)
17:00 Lattice dynamics of PbSe nanostructures
Efterpi Kalesaki (University of Luxembourg, Luxembourg)
17:15 Electronic phase diagram of strongly correlated rare earth materials
Leon Petit (Daresbury Laboratory, UK)
17:30 Concluding remarks from the workshop chairs

17:45 End

Poster Session (Thursday 12:45-14:40 and Friday 12:50-14:00)