

Programme Outline

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"

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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)

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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)

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14:45 *Analysis of energy gap opening in functionalised graphene oxide*

Mark Lundie (University of Salford, UK)

15:00 *Electron irradiation effects on nanomechanical properties of graphene: Molecular dynamics study*

Kazuhiro Tada (Toyama National College of Technology, Japan)

15:15 *Optical and vibrational properties of layered MoS₂*

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 BiVO₄ photoelectrodes for solar water-splitting*

Rachel Crespo-Otero (University of Bath, UK)

16:30 *Step Defects on the TiO₂ 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)