Report on the Collaborative Science & Technology Workshop: "Beyond the Standard: DFT Approaches for the Simulation of Next-Generation Electronics "

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Summary

A workshop on “Beyond the Standard: DFT Approaches for the Simulation of Next-Generation Electronics”, funded by the UCL- French Embassy Collaborative Science & Technology fund, was held on April 13-14th 2015 in the Council Room, University College London. The original aims of the workshop were to:

Explore funding sources for joint collaboration/future group members at each institution.

Researcher exchange: Explore potential for extended stay/collaboration for researchers at each institution.

Research Collaboration: Explore complementarity of research expertise and overlap in research interests to established avenues for collaboration and joint projects/publications.

Expand CONQUEST user base, and explore possibility of expanding developers group along with requirements for new functionality in the code.

Workshop Programme

	Day 1
12:00-12:10	Welcome from CONQUEST Lead Developer Dr David Bowler
12:10-13:00	O(N) DFT in CONQUEST: molecular dynamics and applications David Bowler
13:00-14:00	Lunch
14:00-14:50	Real Time TDDFT: Unitarity, Truncation & Applications Conn O'Rourke
14:50-15:40	Modelling of self-assembled nanostructures for organic electronics Micaela Matta
15:40-16:10	Refreshments
16:10-17:00	Simulation and NMR Spectroscopy of Amorphous Boron Carbide Lionel Tru andier
17:00-17:20	Stress in Conquest Shereif Mujahed
17:20-17:50	The Modern Theory of Polarisation in CONQUEST Kane Shenton
18:00-19:00	Discussion on potential avenues for collaboration & Drinks
19:30	Dinner at the Norfolk Arms, 28 Leigh St, London WC1H 9EP
	Day 2
10:00-10:20	Charge transport in an amorphous triphenylamine- uorene copolymer Sai Manoj Gali
10:20-11:00	Interfaces between organic semiconductors: from structure to charge separation Luca Muccioli
11:00-11:20	Refreshments
11:20-11:40	On nding the density matrix using minimization and puri cation algorithms Mamy Rivo Dianzinga
11:40-12:00	H diffusion and Al doping in Si nanostructures Richard Smith
12:00-12:50	Simulation of second-order nonlinear optical responses of molecular switches Frédéric Castet
12:50-13:10	Water on TiO_2 Jakub Vrtny
13:00-15:00	Lunch & Discussion on avenues for and securing collaborative funding

Participants

UCL

Dr David Bowler Reader in Physics, LCN and Department of Physics & Astronomy, UCL

Research interests: Lead developer of CONQUEST; semiconductor growth; nanostructures on semiconductor surfaces

Dr Conn O'Rourke Research Associate in LCN

Research interests: linear scaling TDDFT; dyes on TiO_2; semiconductor nanowires

Professor Mike Gillan Professor of Physics, LCN and Department of Physics & Astronomy, UCL

Research interests: Accurate, ef cient quantum chemical extensions of DFT; water structure from DFT; quantum Monte Carlo methods.

PhD Students Jakub Vrtny, Richard Smith, Kane Shenton, Shereif Mujahed.

Université de Bordeaux

Dr Lionel Tru andier Assistant Professor, Institut des Sciences Moleculaires, Université de Bordeaux

Research interests: Perturbation theory in linear scaling DFT; NMR calculation in condensed matter

Professor Fréderic Castet Professor, Institut des Sciences Moleculaires, Université de Bordeaux

Research interests:

Future Collaboration

Speci c projects going forward:

Implementation of forces and stresses from exact exchange in CONQUEST. This continues an existing collaboration, extending and improving it. It will greatly increase the usability and international appeal of CONQUEST.

Three month joint visit of Osaka University PhD student (Mr Hirakawa) to Bordeaux and UCL. The overlapping interests of spectroscopy and CONQUEST, along with the extensive UCL-Japan collaboration, have enabled this new initiative to create a new collaboration between these universities.

Royal Society International Exchange application “Simulation of optical properties of polymers using linear scaling DFT approaches”. Dr Bowler and Professor Castet have submitted this grant to fund two years of collaborative visits between UCL and Bordeaux, to apply CONQUEST to calculations of optical properties of polymers. This will bring together the complementary skills of UCL (in method development) and Bordeaux (in polymers) to a new area.

Continuing collaboration between UCL and Bordeaux on the use of CONQUEST for simulations of organic/inorganic interfaces.

Implementation of acceptance testing of all new CONQUEST code based on standard test sets prepared by Dr Tru andier.

Publications

Lionel Tru andier and David Bowler are writing papers on the implementation and testing of exact exchange in CONQUEST (at least two papers—one on the implementation and testing, another on the effects of linear scaling truncation on accuracy and ef ciency of the code)

Lionel Tru andier and David Bowler are also preparing a paper on the implementation of a new approach to idempotency in linear scaling methods

Exchange

David Bowler will visit Bordeaux in September for continuing research collaboration and planning of future visits

Mr Hirakawa of Osaka University will visit Bordeaux

In addition, the Royal Society grant (if successful) will fund three trips to Bordeaux each year (for members of Dr Bowler's group) for two years, and three trips to UCL each year (from Bordeaux) for three years. This will considerably strengthen the links and should lead to several publications, as well as new developments in the code.
Funding In addition to the Royal Society grant already submitted, discussions are underway for submission of a Marie Curie training network involving Bordeaux and UCL, and a three-way link between UCL, Bordeaux and University of Tsukuba, Japan is being explored (building on existing links between Bordeaux and Tsukuba, and UCL and Tsukuba).

Finance

The funds provided were used to pay for travel and hotel accomodation for the Bordeaux visitors, and for the meals at the workshop (lunches, drinks, and the workshop dinner).

Final Remarks

The workshop offered excellent opportunities for discussions of scienti c areas for collaboration, speci c projects and funding that might be pursued. The participants are extremely grateful to the Collaborative Science & Technology fund for the opportunity to hold the workshop, and for the outcomes described here.