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WARWICK
THE UNIVERSITY OF WARWICK

2016-17 Warwick EPSRC Symposium

Density Functional Theory: Analysis and Computation

3-7 July 2017

Organisers: Christoph Ortner (Warwick), Eric Cances (Paris), Gabor Csanyi (Cambridge)

Programme

All lectures will be held in Room B3.03

Monday

10:20 Coffee in the Mathematics Institute Common Room

11:00 **Fred Manby** (Bristol) — *Connecting wavefunctions and density functional theory*

11:40 **Gero Friesecke** (TU-Munich) — *Pair densities in density functional theory*

12:30 Buffet Lunch in the Mathematics Institute Common Room

15:20 **Alessandro De Vita** (KCL) — *Predicting QM-accurate forces for chemo-mechanical materials modelling*

16:00 **Jiangfeng Lu** (Duke) — *Stochastic algorithms for high dimensional quantum systems*

16:40 **Ralf Drautz** (Bochum) — *From density functional theory to magnetic analytic bond order potentials*

18:00 Buffet Dinner in the Mathematics Institute Common Room

Tuesday

09:00 **Roger Haydock** (Oregon) — *An exact independent electron method for interacting electrons*

09:40 **George Booth** (KCL) — *Combining 'Chemistry' and 'Physics' approaches for stronger correlation?*

10:20 Coffee in the Mathematics Institute Common Room

11:00 **Albert Bartok** (STFC) — *Learning interactions from microscopic observables*

11:40 **Faizan Nazar** (UPMC) — *Locality of Electronic Structure Models*

12:30 Buffet Lunch in the Mathematics Institute Common Room

15:20 **Dallas Trinkle** (Illinois) — *Dislocation cores and defect interactions from first principles: Current state of the art and new challenges*

16:00 **Lin Lin** (UC Berkley) — *Green's function embedding*

16:40 **Alexey Sokol** (UCL) — *Point defects in wide-gap semiconductors from hybrid QM/MM embedded cluster calculations*

Continued over

For further information on events at the Mathematics Institute, see: **go.warwick.ac.uk/mathsevents**
or contact: **Mathematics Research Centre, Zeeman Building, University of Warwick, Coventry CV4 7AL, UK**
E-mail: **mrc@maths.warwick.ac.uk** *Phone:* **+44(0)24 7652 8317** *Fax:* **+44(0)24 7652 3548**

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Programme continued

Wednesday

09:00 **Thierry Deutsch** (Grenoble Alpes) *The flexibility of Daubechies wavelets for electronic structure calculations*

09:40 **Genevieve Dusson** (UPMC) *A posteriori error analysis and post-processing methods for linear and nonlinear eigenvalue problems*

10:20 Coffee in the Mathematics Institute Common Room

11:00 **David Gontier** (Paris-Dauphine) *Supercell method for the simulation of insulators without and with defects*

11:40 **Salma Lahbabi** (Casablanca) *A mean-field model for disordered crystals*

12:30 Buffet Lunch in the Mathematics Institute Common Room

15:20 Organised Walk/Free afternoon

Thursday

09:00 **Huajie Chen** (PekingNormal) *Numerical analysis of finite temperature DFT*

09:40 **Antoine Levitt** (ENPC) *Numerical analysis of Brillouin zone integration methods*

10:20 Coffee in the Mathematics Institute Common Room

11:00 **Eric Polizzi** (UMass Amherst) *FEAST-based scalable algorithms for real-space and real-time first-principle calculations*

11:40 **Reinhold Schneider** (FU Berlin) *Combination of tensor networks (QC-DMRG) with a coupled cluster method*

12:30 Buffet Lunch in the Mathematics Institute Common Room

15:20 Short talks by Students and Postdocs

18:30 Conference Dinner at The Cross, Kenilworth

Friday

09:00 **James Kermode** (Warwick) *Multiscale modelling of rare events in materials chemomechanics*

09:40 **Daniel Urban** (Fraunhofer Munich) *DFT inspired materials design: Towards Z phase-strengthened 12% Cr ferritic-martensitic steels*

10:20 Coffee in the Mathematics Institute Common Room

11:00 **Yvon Maday** (UPMC) *Title tba*

11:40 **Garnet Chan** (Caltech) *Representations and complexity of classical and quantum simulations of electronic structure*

12:30 Buffet Lunch in the Mathematics Institute Common Room