Electronic Structure Theory

Justification for existence

First principles calculations of materials designed to *complement* experiments, by

- helping to understand results of real experiments,
- calculating things that are experimentally inaccessible or cost too much money,
- providing an atomic scale resolution beyond most experiments,
- calculating things which don't exist (in experiments usually stuck with lowest free energy phase unless there is large activation energy so that metastable phases can be studied),

by solving the Schrödinger equation entirely from first principles with no adjustable parameters.

PLUS since we can only do this approximately, we try to

- improve the approximations to get better accuracy,
- improve the speed and scaling behaviour of the algorithms

PLUS, as a service to the scientific community,

- we write generally applicable computer codes which do all of the above.

Electronic Structure Research Activities

Techniques: density functional theory, Hartree-Fock theory, molecular dynamics, quantum Monte Carlo, occasional quantum chemistry methods.

Code and algorithm development

- CASINO : Quantum Monte Carlo code
- CASTEP : DFT plane wave code
- ONES : $\mathcal{O}(N)$-scaling DFT code

Other codes used in TCM for applications

- CPMD - DFT ab initio MD (Car-Parrinello)
- CRYSTAL - DFT/Hartree-Fock local basis set code
- PARATEC - DFT plane wave code
- GAUSSIAN - Monolithic quantum chemistry package

Methods development:

$\mathcal{O}(N)$-scaling DFT and QMC(!) ; NMR chemical shifts ; core-level spectra ; pseudopotential development ; linear optical properties ; etc..

Applications

biological systems ; strongly correlated systems and magnetism ; manganite physics ; electron gas and electron-hole systems ; polarization, localization and metal-insulator transitions ; systematic prediction of crystal structures ; polymers and organic electronic devices ; grain boundaries ; etc..

TCM Electronic Structure Theory

Mike Payne

Postdocs: Chris Pickard, Oswaldo Dieguez, Chris Skylaris, Peter Haynes, (Matt Segall)
Old students: Roger Chen, Sian Joyce, Arash Mostofi, Jonathan Yates
New students: [fill in here]

Richard Needs

Postdocs: Mike Towler, Ryo Maezono
Old students: Yoonseok Lee, Martin Vogt, Simone Chiesa (1 year visit)
Strays: Valeria Ferrari, Gavin Brown
New students: [fill in here]

Carla Molteni

Students: Brent Walker
New students: [fill in here]

Various sorts of professor etc. who turn up at the ESDG

Neil Ashcroft, Emilio Artacho, Volker Heine