Institution: University of Durham

Unit of Assessment: 9/Physics

Title of case study: Commercialisation of materials modelling software (**Castep**)

1. Summary of the impact

Durham researcher, Prof Stewart Clark, is one of the six original co-developers of the Castep software package which calculates the electronic, physical and chemical properties of materials from first principles. Castep was written to solve a variety of research problems from semiconductor devices and liquid crystal displays, to the behaviour of Earth minerals under very high pressure, molecular dynamics and biological systems. The software package was commercialised for use in industry under license by Accelrys Inc., where it is bought and used by ~1000 high-tech companies for development of new materials in chemical, pharmaceutical, auto and jet engine manufacturing industries. Total sales revenue for Accelerys from the Castep code is in excess of $30M.

2. Underpinning research

The properties of materials can be predicted from first principles from their electronic structure, but these are prohibitively time consuming to calculate from a basic wavefunction approach. Instead, density functional theory is a much more powerful technique to solve many body problems in quantum mechanics (winning the 1999 Nobel prize for Walter Kohn). This gives the energy levels and wavefunction of the material, but the more useful information is how it responds e.g. to light, phonons, neutrons etc as this is directly measureable and has a direct connection to applications for the material. Typically this response is determined by the second derivative of the energy, which requires perturbative methods. In the late 1990s there were existing codes which used the density functional approach to calculate wavefunctions and energies, but these were all developed for specific applications by multiple authors and were not efficient enough to extend to perturbation theory. They were also typically poorly documented, and difficult to port onto the new parallel computing environments which were beginning to appear.

Prof Stewart Clark (member of Durham Physics Department 1997-present), together with a small group of theoretical condensed matter physicists, decided that the lack of efficient computational tools was a serious barrier to their research and that they should build a new code from the ground up. Their code was fundamentally designed to run on parallel machines, and be fully documented so that additional functionality could easily be incorporated by external researchers as well as the authors. The original CASTEP Developers Group consisted of Stewart Clark (Durham), Phil Hasnip, Mike Payne and Chris Pickard (Cambridge), Matt Probert (York) and Matt Segall (now in industry). While these are all credited as equal co-authors, Prof Clark's contribution included development of the new, efficient computational implementation of the density functional theory which forms the heart of the CASTEP code [1-2]. He also developed a new, much more computationally efficient way to solve the non-local interactions between electrons [3], which he has recently updated [4].

The first public release of CASTEP was in 2001, and Prof Clark immediately used this to tackle his research problems, including how to circumvent the miniaturization limit for transistors. Standard silicon dioxide materials hit a quantum limit below 22 nm as electrons start to tunnel through the transistor gate so the device is no longer a reliable switch. Prof Clark used CASTEP to calculate the properties of numerous alternative semiconductor materials, and showed that quantum tunnelling was much less of an issue for Halfnium dioxide, so chips made using this material could be made much smaller [5]. The same year, Intel independently released its first chip based on Halfnium dioxide, demonstrating that this did indeed allow miniaturization as predicted by CASTEP.

Another research project was with multi-ferroic materials. In general, materials can be either ferro-magnetic or ferro-electric but not both as ferro-magnetism occurs when spin degeneracy is lifted by pushing electrons to unfilled states, whereas ferro-electric materials push electrons towards filled states so the two are generally mutually exclusive. However, a very small number of materials do show both, and these are very important both for the intriguing science underlying the phenomena, and the exciting potential of devices where both the magnetic and charge properties can be controlled. Of these, $BiFeO_3$ is one of the few to exhibit this behaviour at room temperature, as required for device applications. Prof Clark was able to use CASTEP to explain how the

electronic structure of $BiFeO_3$ allowed this to happen. This fundamental understanding of the underlying physics is a prerequisite to precise control of the behaviour of the material in spintronics (magnetic switching) devices [6].

CASTEP can also tackle fundamental issues in biology such as the topology of molecular networks. These are extremely difficult to calculate but critically determine all the material properties, including chemical bonding and crystallization. Prof Clark was able to use CASTEP's accurate electronic structure calculations to predict the three major crystalline structures of glycine, the first amino acid for which this was possible, and to show that another could exist at higher pressure [7].

The Developers Group continuously update the code to add functionality such as modules to calculate the results of Raman spectroscopy and nuclear magnetic resonances. This makes the code a unique resource, allowing communication and collaboration between experimentalists and theorists, in both industry and academia, increasing its impact and scope significantly.

Over 4000 peer-reviewed publications across a wide range of disciplines have used the code. It is also used in training highly skilled graduate students, many of whom have gone on to work in industry. Several hundred PhD theses from 2002 to the present have been based on calculations using CASTEP, contributing to the large number of scientific papers published in leading peer reviewed international journals.

3. References to the research

[1] *First principles methods using CASTEP*, SJ Clark, MD Segall, CJ Pickard, PJ Hasnip, MIJ Probert, K Refson, MC Payne, Zeitschrift für Kristallographie 220, 567, 2005
Over 1400 citations

[2] *First-principles simulation: ideas, illustrations and the CASTEP code*, MD Segall, PJD Lindan, MJ Probert, CJ Pickard, PJ Hasnip, SJ Clark, MC Payne, Journal of Physics: Condensed Matter 14 (11), 2717, 2002
Over 3500 citations

[3] *Variational density-functional perturbation theory for dielectrics and lattice dynamics*, K Refson, PR Tulip, SJ Clark Physical Review B 73 (15), 155114, 2006
Over 140 citations

[4] *Optimized effective potential using the Hylleraas variational method*, TW Hollins, SJ Clark, K Refson, NI Gidopoulos, Physics Review B, 85, (23), 235126, 2012

[5] *Defect energy levels in HfO2 high-dielectric-constant gate oxide*, K Xiong, J Robertson, MC Gibson, SJ Clark, Applied Physics Letters 87 (18), 183505, 2005
Over 230 citations

[6] *Beta phase and gamma-beta metal-insulator transition in multiferroic $BiFeO_3$* R Palai, RS Katiyar, H Schmid, P Tissot, SJ Clark, J Robertson, SAT Redfern G Catalan, JF Scott, Physical Review B 77 (1), 014110, 2008
Over 220 citations

[7] *Effect of high pressure on the crystal structures of polymorphs of glycine*, A Dawson, DR Allan, SA Belmonte, SJ Clark, WIF David, PA McGregor, S Parsons, Crystal Growth & Design 5 (4), 1415, 2005
Over 100 citations

4. Details of the impact

CASTEP can be used to simulate a wide range of materials including crystalline solids, surfaces, molecules, liquids and amorphous materials. It can calculate the properties of any material that can be thought of as an assembly of nuclei and electrons with the only limitation being the finite speed and memory of computers systems [C1, see Fig 1]. Applications include:

- Device technologies: modelling materials for new semiconductor devices including

nanoparticles, high dielectric constant materials, data-storage materials
- Geology: elastic, thermal and dynamical properties of Earth and planetary material under extreme conditions
- Spectroscopy: Interpretation of experimental studies in a wide variety of spectroscopic techniques such as Raman, Infra-red, nuclear magnetic resonance, electron energy loss spectroscopy, neutron spectroscopy
- New light emission materials: Investigations on liquid crystals, light emitting polymers, light emitting semiconducting materials all used in new display technologies
- Structure prediction: investigations of the structures of new materials ranging from pharmaceuticals and life-science molecules to semiconductors, spintronics and complex metals.

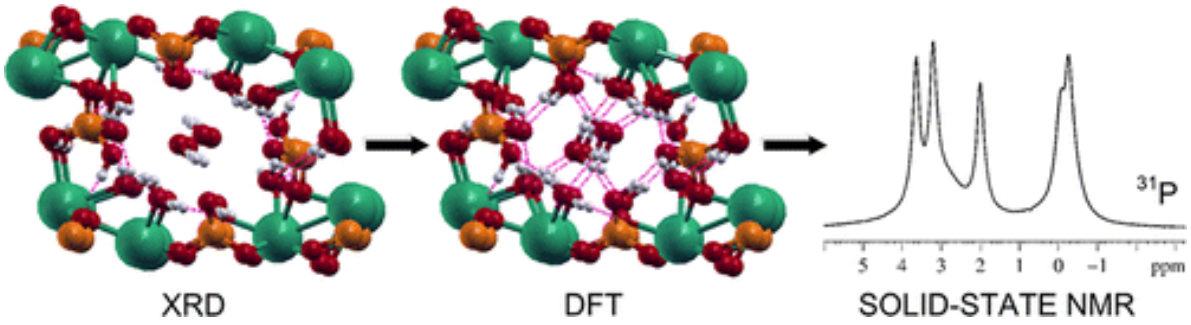

Fig 1. Example CASTEP output exploring biomineralisation of octacalcium phosphate (OCP), a precursor phase in bone mineral formation. This shows X-ray crystallography, first-principles density functional theory calculations, and solid-state nuclear magnetic resonance spectroscopy predictions of the structure.

The reputation of the code was such that the authors were approached by Accelrys Inc, a NASDAQ-quoted research and development software company based in San Diego, USA, which employs over 360 people and has an annual turnover of $81M [C2]. They proposed licensing the software so they could market it for scientific, industrial and technological applications. Accelrys incorporated CASTEP into its Materials Studio modelling and simulation platform which has been bought by over 800 companies worldwide [C3], making this the best selling software package of its type. These include some of the largest manufacturers in the chemical (e.g. Unilever), pharmaceutical, automobile (e.g. Toyota, General Motors) and aviation (e.g. Boeing) sectors, as well as smaller scale high-tech science companies, testifying to the commercial viability of the product across a wide spectrum of business sizes and sectors [C3].

Research into the effectiveness of CASTEP, sponsored by Accelrys, found that customers were able to recoup their investment in software tools up to ten times over. The major cost savings in applying computer simulations to the research and development of materials were from circumventing the need for costly experiments and shorter developmental timescales.[C4]

The code is deeply embedded in industry, so its full impact is not possible to quantify, especially as much of the information is commercially sensitive. However, an Accelerys survey of patents based on CASTEP shows that 83 have been published since 2008 [C5]. Examples include one filed by the Tokyo-based OKI Electric Industry Co. Ltd which is pioneering a method of forming a gate recess in a semiconductor device. Another of the patents was issued in 2010 to the German-US chemicals giant Kronos International Ltd for an invention relating to titanium dioxide pigment particles and methods for their manufacture.

Sales of Castep are producing an annual return of £2.5m to Accelerys, with total sales in excess of $30M [C3]

5. Sources to corroborate the impact

C1 Castep web site
http://www.castep.org

C2 Accelrys company information
http://www.cbronline.com/companies/accelrys_inc

C3 Accelerys letter of support
Filed with supporting documents

C4 Materials Studio cost reduction
http://accelrys.com/products/materials-studio

C5 Patents report
Filed with supporting documents