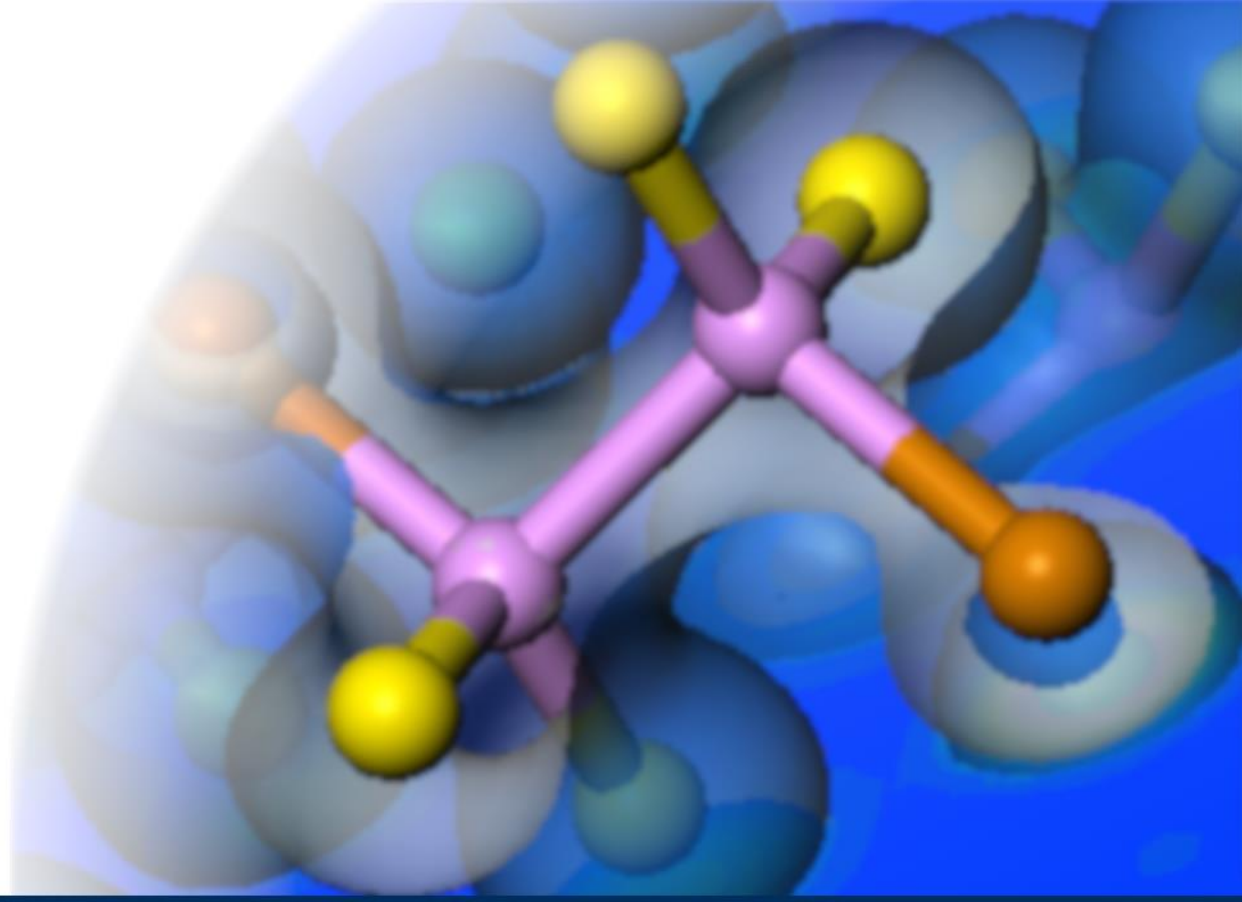
CASTEP



A Brief History of CASTEP

Dr Matthew Segall – Optibrium Limited (TCM 1994-2003)

What is CASTEP?

CAmbridge
Serial
Total
Energy
Package

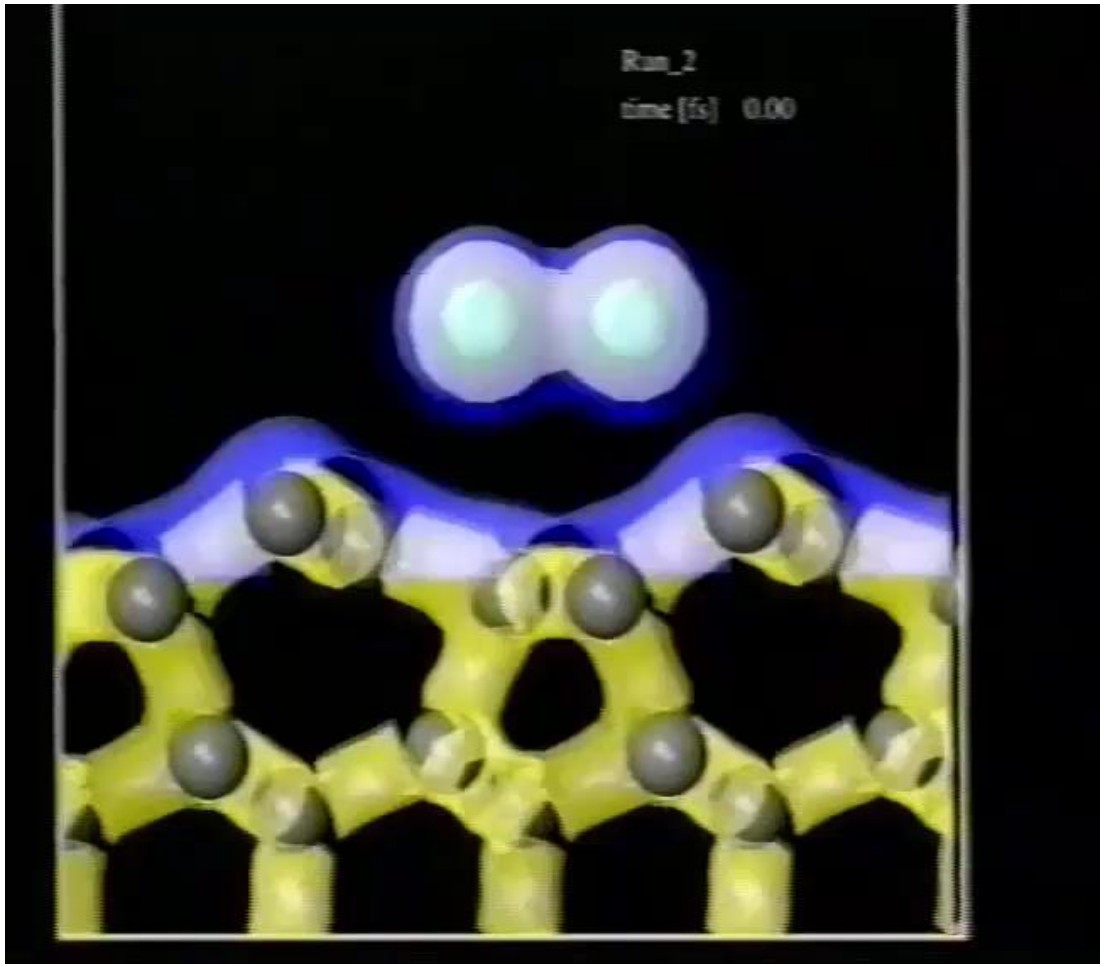
- Materials modelling code
  - Density Functional Theory
  - Plane wave pseudopotentials
- Extensive capabilities for simulation of
  - Energetics
  - Structure at an atomic level
  - Vibrational properties
  - Electronic response
  - Spectroscopy
- www.castep.org

Example Applications of CASTEP

Dissociative chemisorption of chlorine molecule on the (111) surface of silicon.

Ab initio molecular dynamics simulation

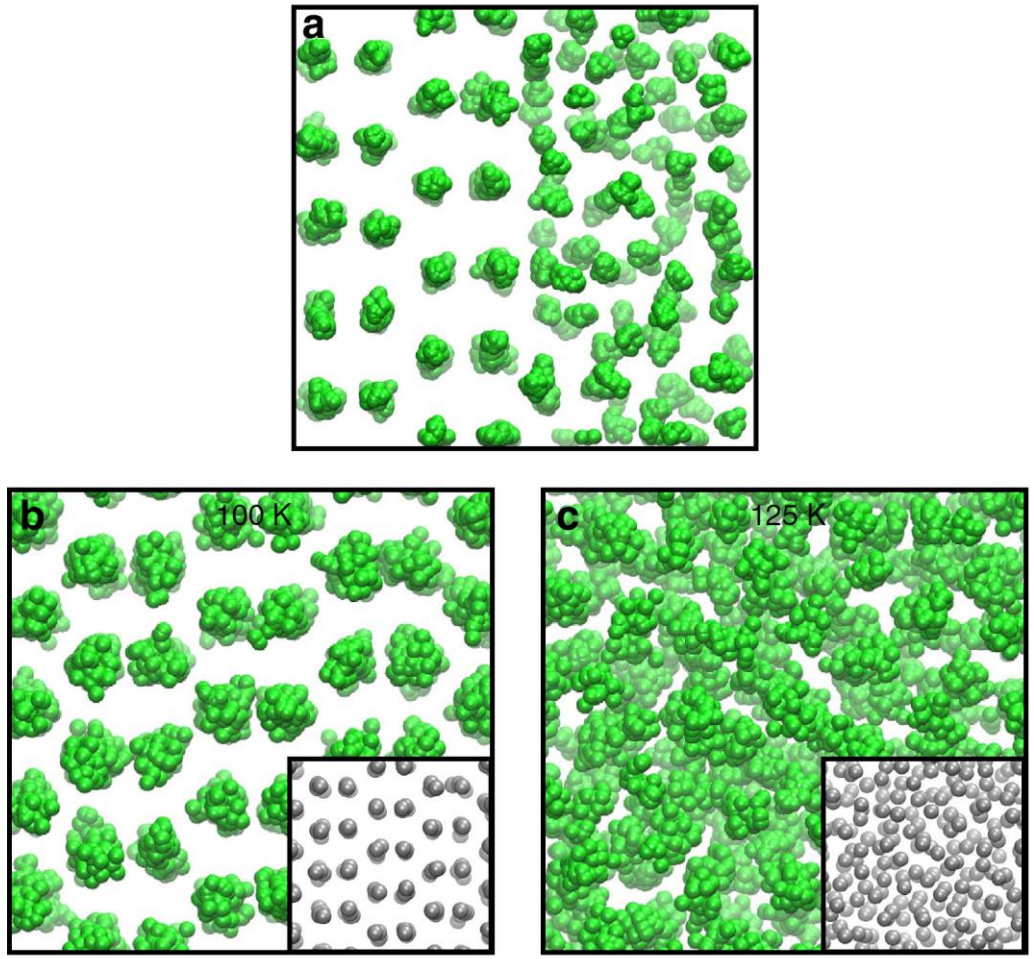
De Vita *et al.* Phys. Rev. Lett. **71**(8) p. 1276 (1993)



Example Applications of CASTEP

Two-phase path integral molecular dynamics simulation of the melting of hydrogen under high pressure.

Chen *et al.* Nature Comms. **4** Article No. 2064 (2013)

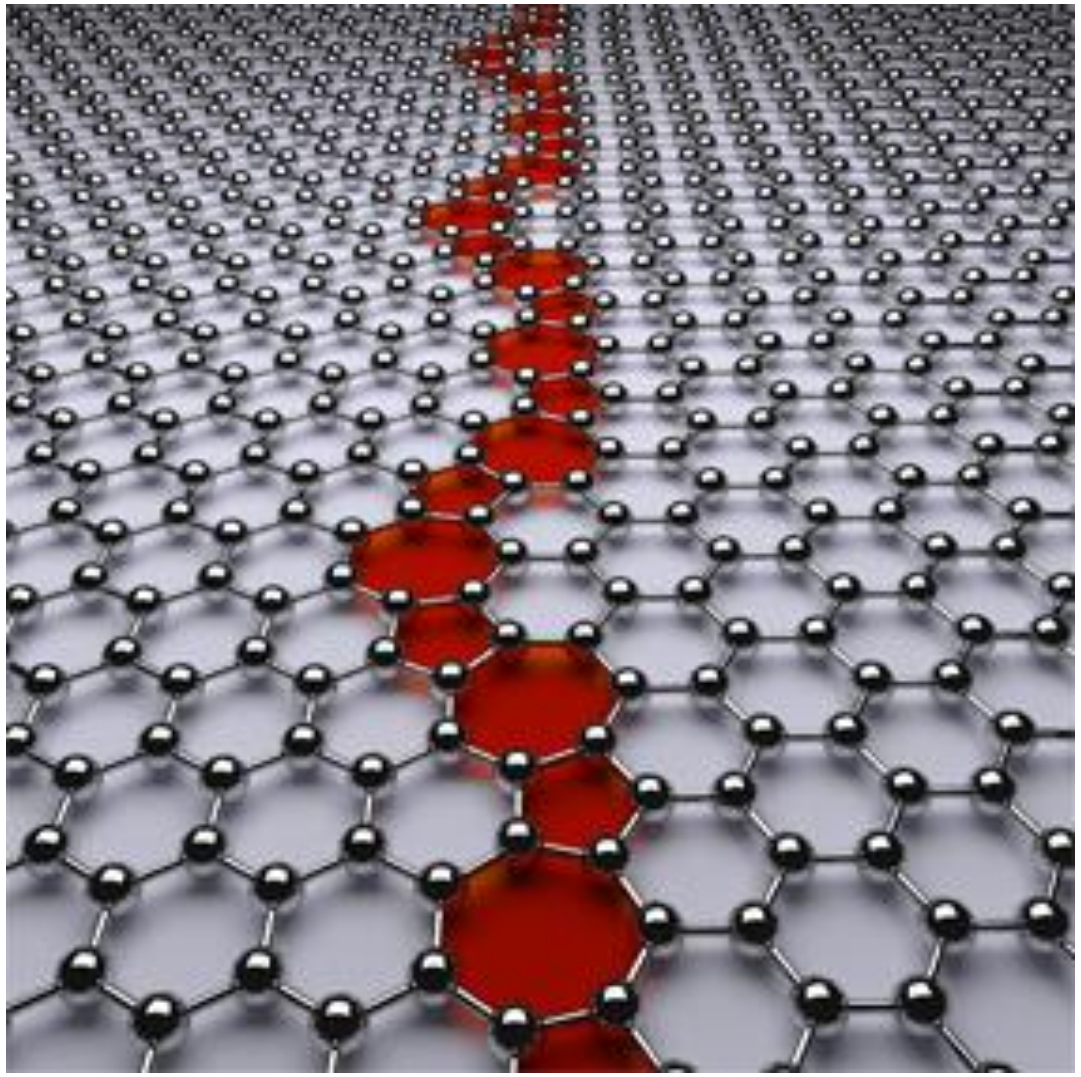


Example Applications of CASTEP

Graphene grain boundary structure between armchair and zigzag regions. The red transparent region marks the interface between the two grains, forming a continuous chain of pentagons and heptagons in the otherwise pristine graphene.

Produced with the Ab initio Random Structure Searching (AIRSS) code and CASTEP.

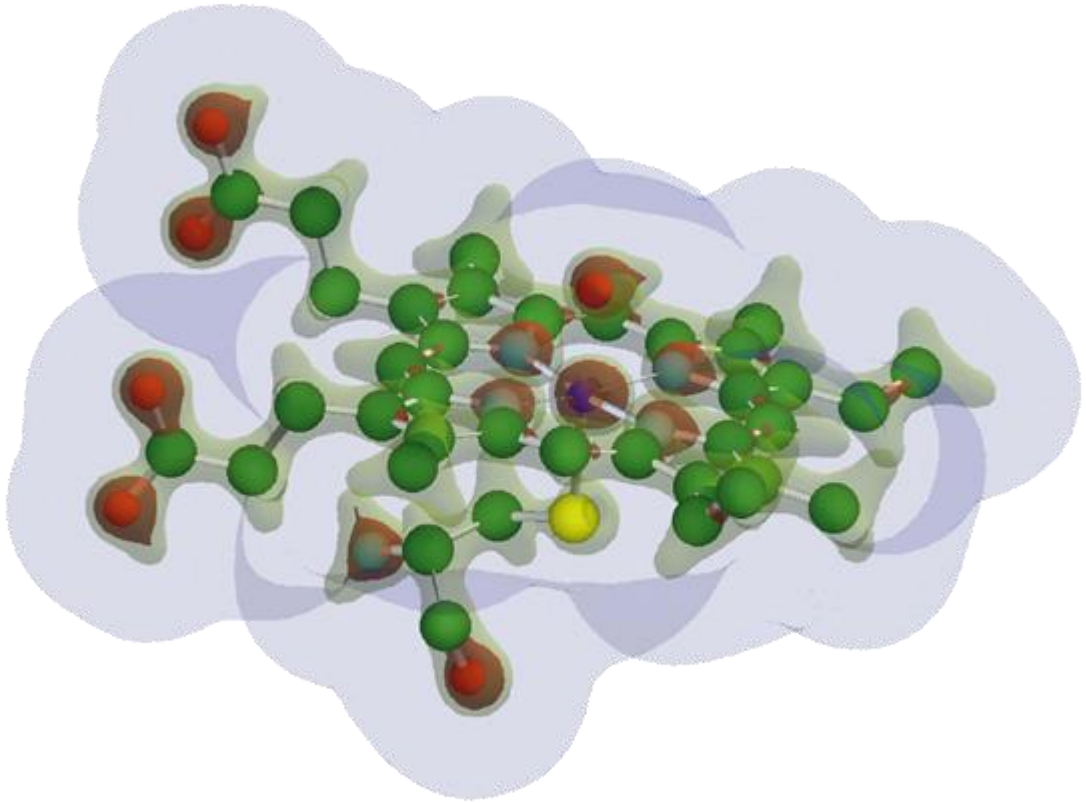
Schusteritsch and Pickard, Physical Review B, **90**(3), Article No. 035424 (2014)



Example Applications of CASTEP

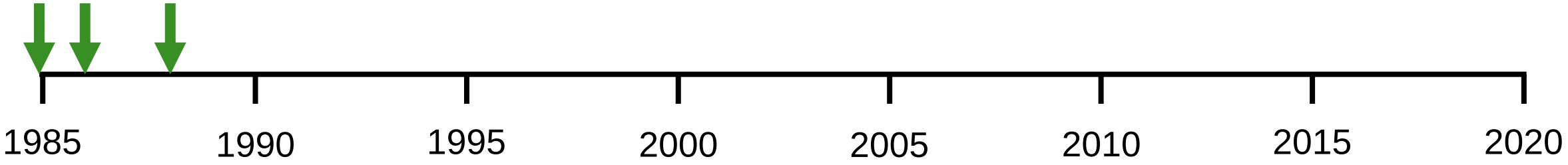
The catalytic centre of Cytochrome P450 drug-metabolising enzymes.

Segall *et al.* Xenobiotica **28**(1) pp. 15-19 (1998)



The Development of CASTEP

The early years



1985

- Mike begins work on a Car-Parrinello code while in John Joannopoulos's group at MIT

1986

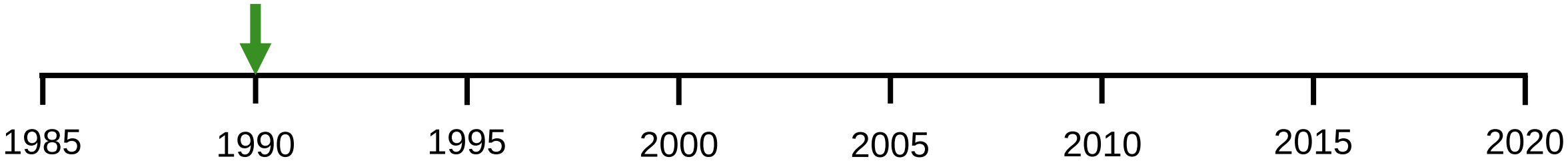
- Mike returns to Cambridge

1988

- The, as yet unnamed, code becomes a CCP9 Flagship Project

The Development of CASTEP

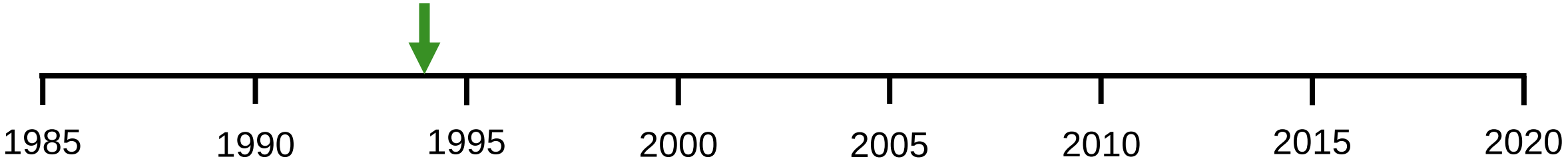
First release



1990

- First release at a CCP9 Summer School
- CASTEP gets its name in a meeting involving Mike, Richard Needs, Karel Kunc and Volker Heine
- A new branch, CETEP, is created by Lyndon Clark at EPCC to parallelise the code

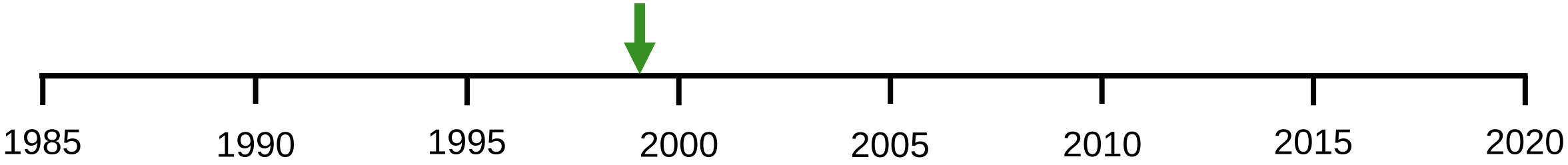
The Development of CASTEP
Commercialisation



1994

- CASTEP is licensed to Molecular Simulations Inc. (MSI)
- Over the years, MSI became Accelrys and then Dassault Systemes (Biovia)

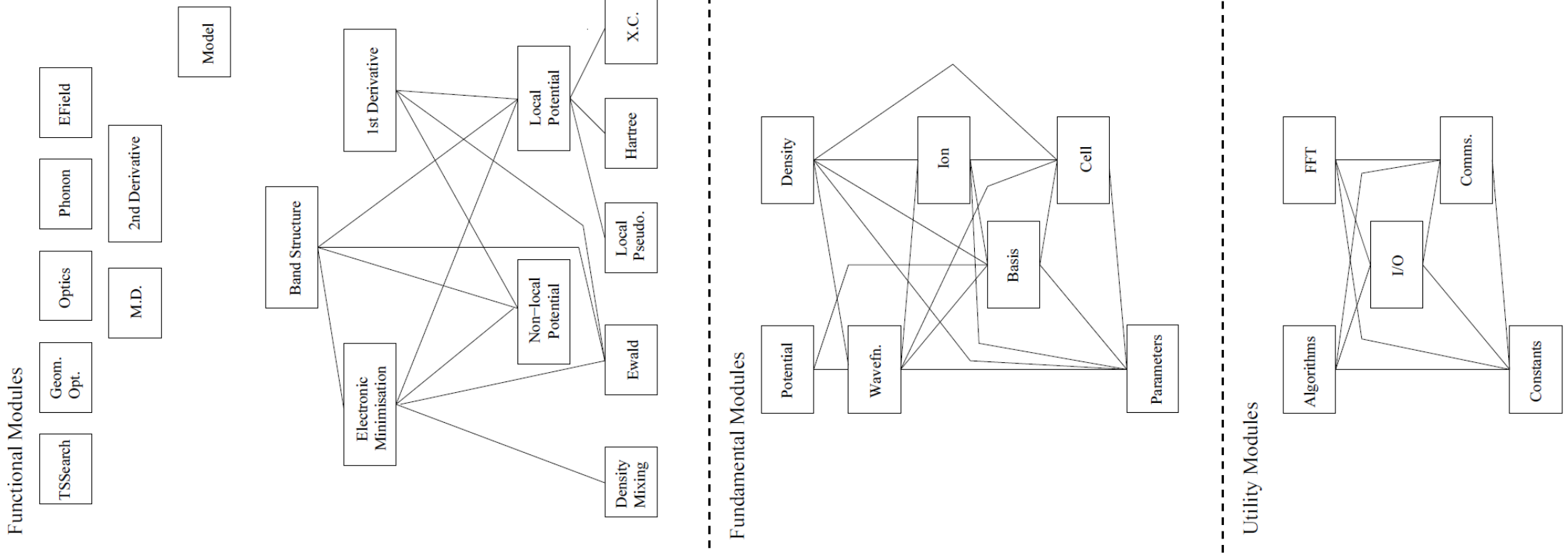
The Development of CASTEP
The genesis of ‘New CASTEP’



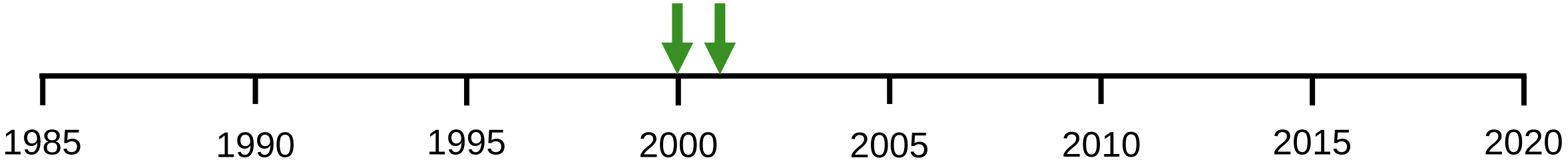
1999

- A group of CASTEP users and developers gather in London to discuss the future of the code
  - Stewart Clark, Phil Hasnip, Phil Lindan, Chris Pickard, Matt Probert, Matt Segall
- We agree to begin work on the specification of a new plane wave, pseudopotential code, ‘NewTEP’

NewTEP Specification



The Development of CASTEP
New CASTEP



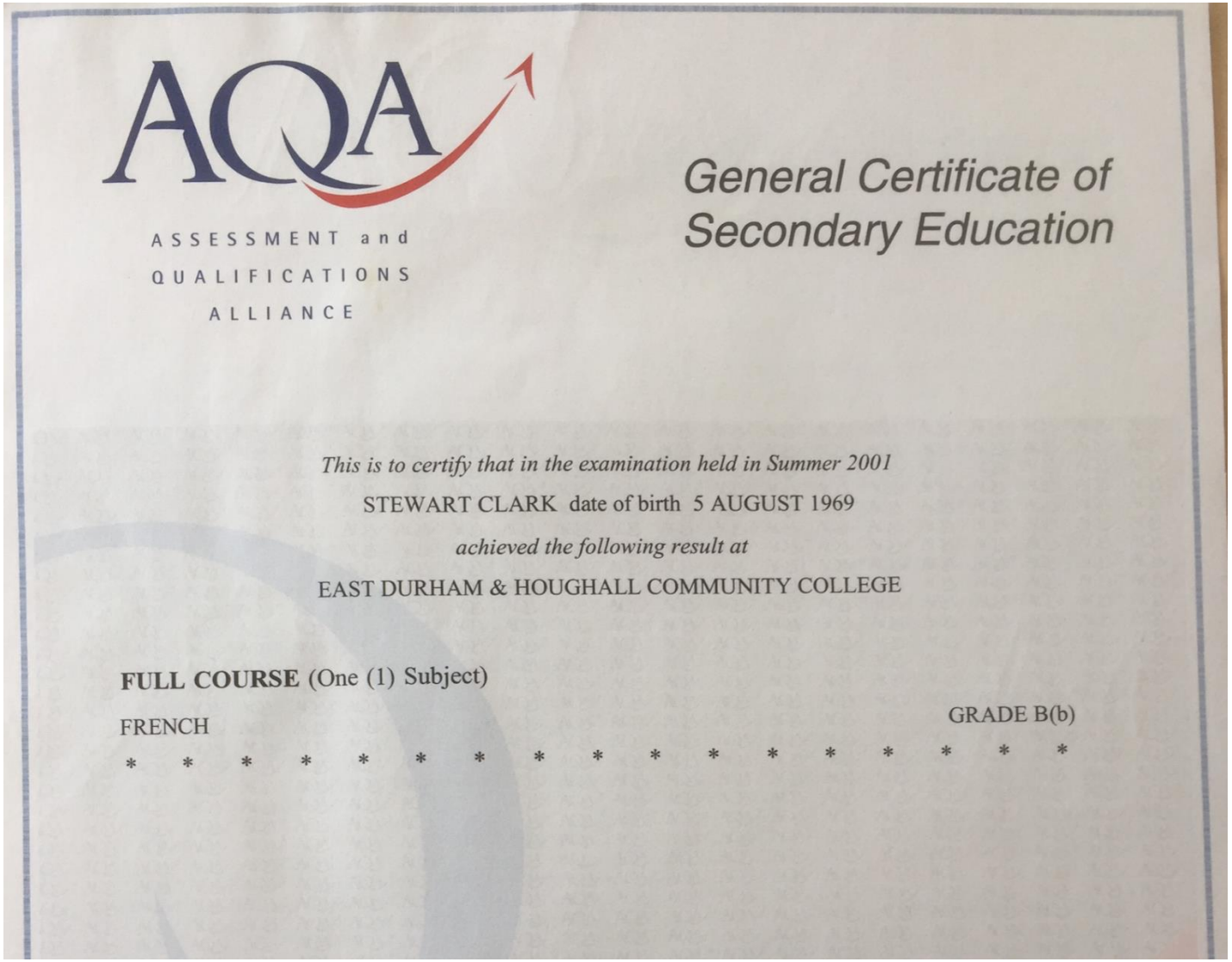
2000

- Implementation begins
- CASTEP Developers Group (CDG) formed
  - Keith Refson joins the group
- Agreement reached with MSI to develop ‘New CASTEP’

2001

- First ‘working’ version completed
- First CASTEP workshop held

Another Achievement Along the Way



AQA

ASSESSMENT and QUALIFICATIONS ALLIANCE

General Certificate of Secondary Education

This is to certify that in the examination held in Summer 2001

STEWART CLARK date of birth 5 AUGUST 1969

achieved the following result at

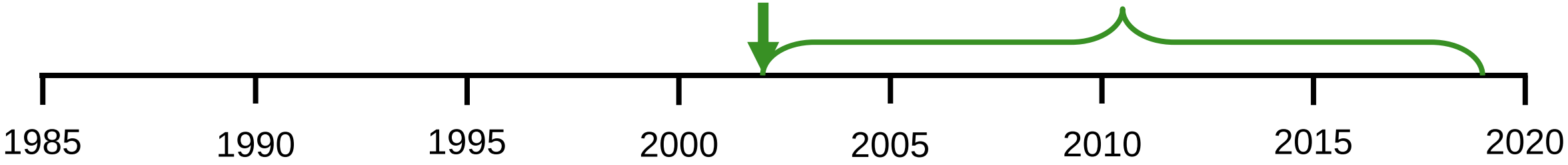
EAST DURHAM & HOUGHALL COMMUNITY COLLEGE

FULL COURSE (One (1) Subject)

FRENCH GRADE B(b)

* * * * * * * * * * * * * * * * * *

The Development of CASTEP
New CASTEP



2002

- First commercial release of New CASTEP

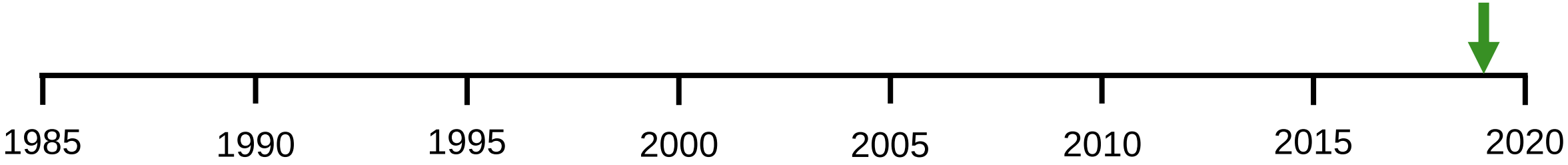
2002 – 2019

- Many new capabilities added…
  - Phonon linear response and finite difference, electric field responses, NMR, EPR/ESR, Wannier functions, non-local/hybrid XC functionals, non-colinear spins, non-linear optics…
- Numerous CASTEP workshops and code fests
- Jonathan Yates joins the CDG

The CDG in Action…

The CDG in Action…

The Development of CASTEP
New CASTEP



2002

- First commercial release of New CASTEP

2002 – 2019

- Many new capabilities added…
  - Phonon linear response and finite difference, electric field responses, NMR, EPR/ESR, Wannier functions, non-local/hybrid XC functionals, non-colinear spins…
- Numerous CASTEP workshops and code fests
- Jonathan Yates joins the CDG

2019

- Renewed agreement with Dassault Systemes to distribute CASTEP

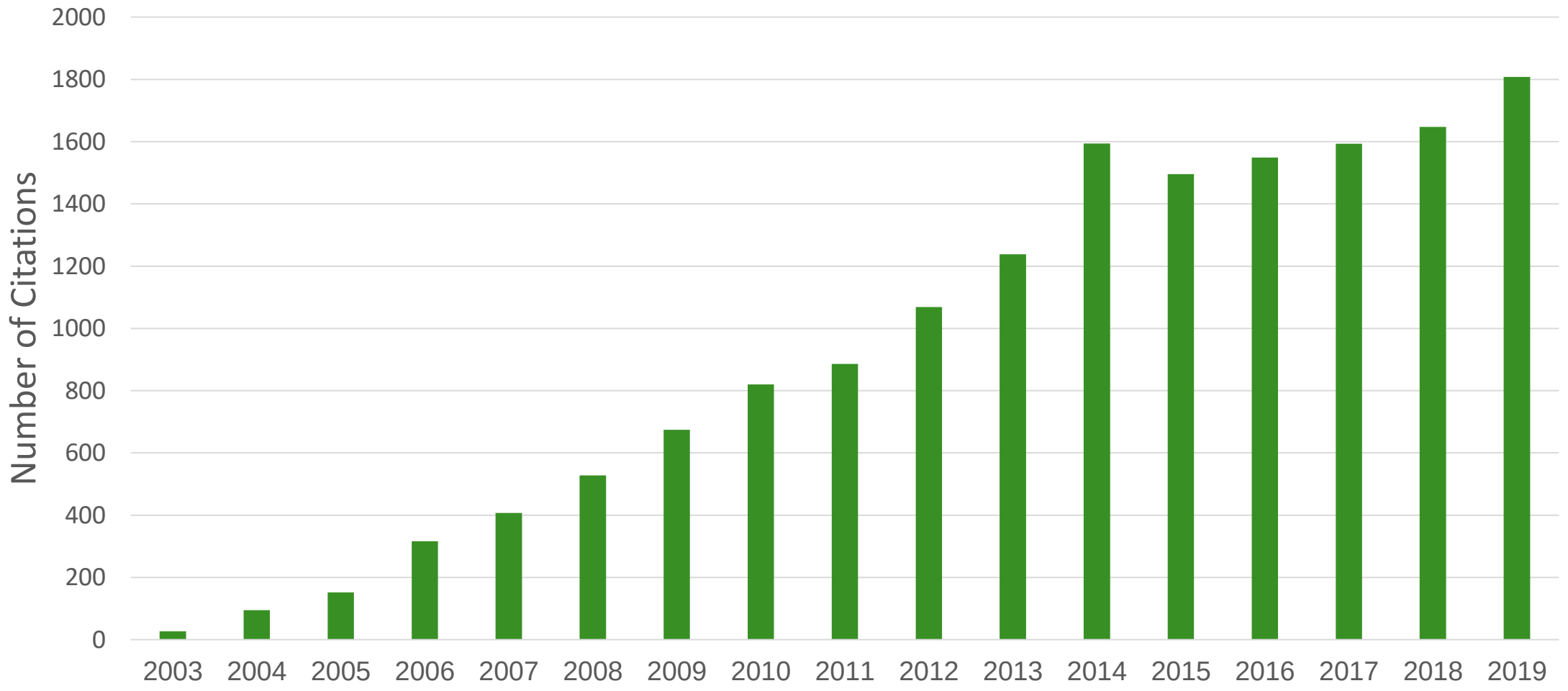
CASTEP is Free for Academic Use

- As a consequence of the new distribution agreement with Dassault Systemes, CASTEP is now available free of charge for academic use
- Under this new license CASTEP has already been distributed to 73 academic groups in 27 countries on all continents (except Antarctica)
- For more information, please contact Dominik Jochym (dominik.jochym@stfc.ac.uk)
- An automated process for license application and download is being prepared

The Principles of CASTEP

- Robustness
  - It should ‘just work’ for any physically reasonable input
- Consistency
  - All code paths should work to the extent supported by theory
- Accuracy
  - The default parameters should give an accurate result
- Efficiency/Speed
  - Highly optimised, excellent parallel efficiency and soon GPU support
- Developability
  - Well-documented, high-quality code

CASTEP's Impact



Google Scholar: J. Phy. Cond. Matt. 14(11) p. 2717 (2002) and Zeitschrift fuer Kristallographie 220(5-6) p. 567 (2005)

Programming vs Software Engineering

CASTEP

Programming

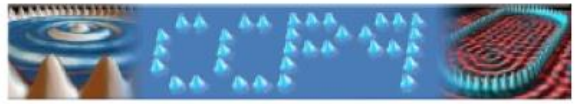
- Individual pursuit
- Works for my application
- May fail with unexpected input
- Works now

Software Engineering

- Coordination among a group
- Robust for general application
  - Testing
- Gracefully handles exceptions
- Maintainable in the long term
  - Built with future development in mind

Acknowledgements

- Mike Payne
- The CASTEP Developers Group
  - Stewart Clark
  - Phil Hasnip
  - Chris Pickard
  - Matt Probert
  - Keith Refson
  - Jonathan Yates
- The many other contributors to CASTEP over the decades
  - Sorry there isn't room to name you all!



Computational Electronic Structure of Condensed Matter

UKCP

BIOVIA