Analysis of results

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Overview

- Lecture III: Analysis of results
  - At the end of a calculation . . .
  - Atomic structure and energy
  - Electronic structure
  - Population analysis
  - Application: theoretical strength and cleavage of diamond

At the end of a calculation . . .

- You've loaded your structure, hit "go" and the computer has done its work
- Now what?
- Are your results *converged*?
  - super-cell
  - cutoff energy
  - **k**-points
- If so — you have lots of potentially useful data on your hard-disk

" If you know the wavefunction, you know everything there is to know about the system"

Simulation vs. analysis

- Simulation
  - calculate a property observed experimentally
- Computer experiments
  - calculate properties that are not necessarily observable, but increse understanding of the system

Atomic structure and energies

- Ground state geometry
- Phase transitions under pressure
- Relative stabilities
- Reaction energy barriers
- Molecular dynamics — temperature
- Phonons

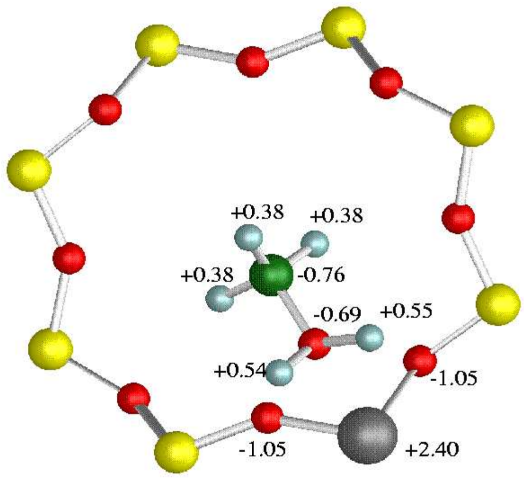
Electronic structure

- Look at the wavefunctions and energy levels
- Densities of states
- Metal/semiconductor/insulator
- Excitations
  - optical properties (colour)
- More in the next lecture

Population analysis

- Wavefunctions hard to interpret
- Quantum Chemical approaches in terms of localised orbitals allow more straightforward interpretation
- Planewaves are nowhere in particular
- Project them onto local orbitals and do population analysis
  - electrons per atom
  - electron per bond
- Qualitative only

Methanol in Zeolites



Mulliken charges for methanol adsorbed in an 8 ring of a zeolite structure

M.D. Segall, C.J. Pickard, R. Shah, and M.C. Payne. Population analysis in plane wave electronic structure calculations. *Molecular Physics*, 89(2):571-577, 1996.

Theoretical strength and cleavage of diamond

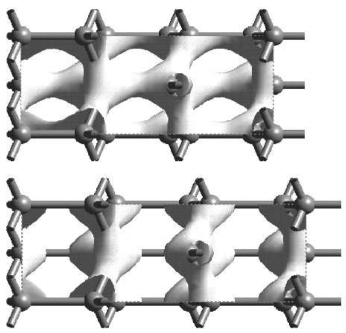
- For centuries, diamond polishers have noted that diamonds cleave easily when struck by a well oriented blow
- Fracture occurs along a preferred set of planes, the $\{111\}$ planes
- A definitive explanation had not emerged

Previous attempts ...

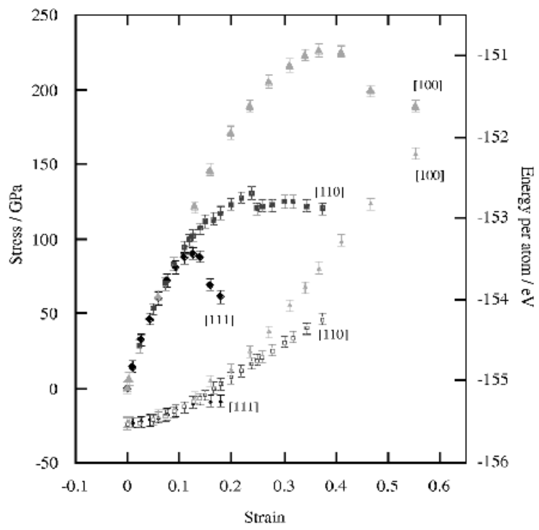
- Surface energy calculated by number of cut bonds
  - $\{111\}$ weakest, but energy differences too small
- Use semiempirical approaches
  - same story
- Invoke impurities

A first principles approach

- DFT can handle structural properties well
- Equally good under extreme conditions (in contrast to more empirical approaches)
- Simply take a unit cell of diamond and stretch it in different directions and see when it breaks . . .



Theoretical breaking stresses



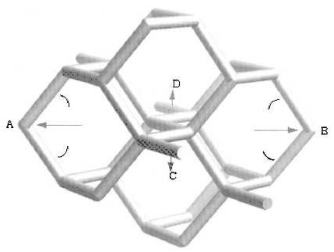
R.H. Telling, C.J. Pickard, M.C. Payne, and J.E. Field.

The theoretical strength and cleavage of diamond.

Physical Review Letters, 84(22):5160-5163, May 2000.

It worked!

- {111} lowest theoretical breaking stress
- Energy to fracture significantly lower
  - {100}:{110}:{111} 7:2.8:1
  - 1.73:1.22:1 by bond counting
- Can be understood in terms of bond bending vs. stretching
- Conclusion: the anisotropy is an *intrinsic* property of diamond



A model first principles study

- Identify a problem (hopefully of interest)
- Can first principles help resolve it?
- Find the simplest realistic model
- Analyse the results
- Understand the results