Session 2:
Thermodynamics, Statistical Mechanics, and Excited States from First Principles

Chair: Matthieu Verstraete

CECAM Multiscale Sep 9 2013 PM

Platja D'Aro

The session

Jörg Neugebauer

« Get the thermodynamics right! »

- High impact steels
- Thermodynamic sampling efficiency lacking
- Novel sampling methods

The session

Karsten Reuter

« Your solid is not alone! **»**

- Surface/interface effects with liquid/gas
- Effects on catalysis (esp. at surfaces)
- Integration of microkinetics in fluid dynamics

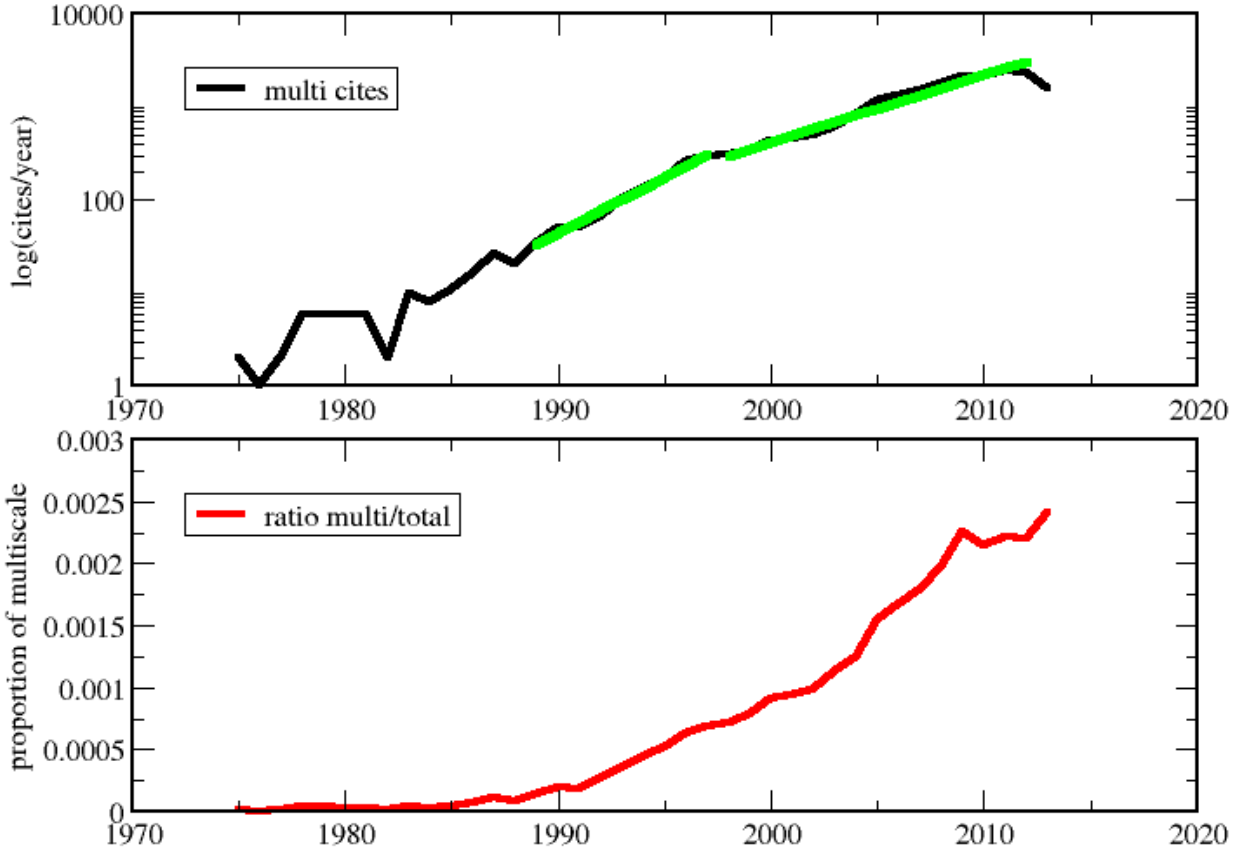
The session

Claudia Ambrosch Draxl

« DFT is not enough! »

- Spectroscopic/optical calculations
- Bethe-Salpeter equation
- Extend this to (at least) DFT problem sizes

How popular is multiscale?



scopus 9/9/2013

Information science

- How to convey information to next level of coarseness?
- How much to convey?
  - position dependence?
  - structural dependence, anisotropy?
  - temperature, chemical potential dependence?
- Choice is critical and non-trivial in ½ of the cases
  - transport coefficients (clear choice of continuum model)
  - local structural effects (many choices for MM)

Questions for speakers (and everyone)

At meso/macro scale quantum details are averaged out:
this is what we want, BUT -

- what are we bringing if we then average out?
- wrt reaction / dielectric contants fit to experiments?
- ab-initio confined to « explaining » not predicting?

- Go beyond PES sampling to other properties?

Questions for speakers (and everyone)

- Can you bridge more than 2 length scales?
- Micro to meso or micro to continuous is easy
  - nanostructure / electrons
  - microstructure, texturing
  - dislocations, cracks, complex disorder
  - mesostructure, contacts, bonding
  - macrostructure, casings, environment...
- Multi means more than 2!
- Can you couple the coarse environment back?