Nanoscience/technology and Software Development

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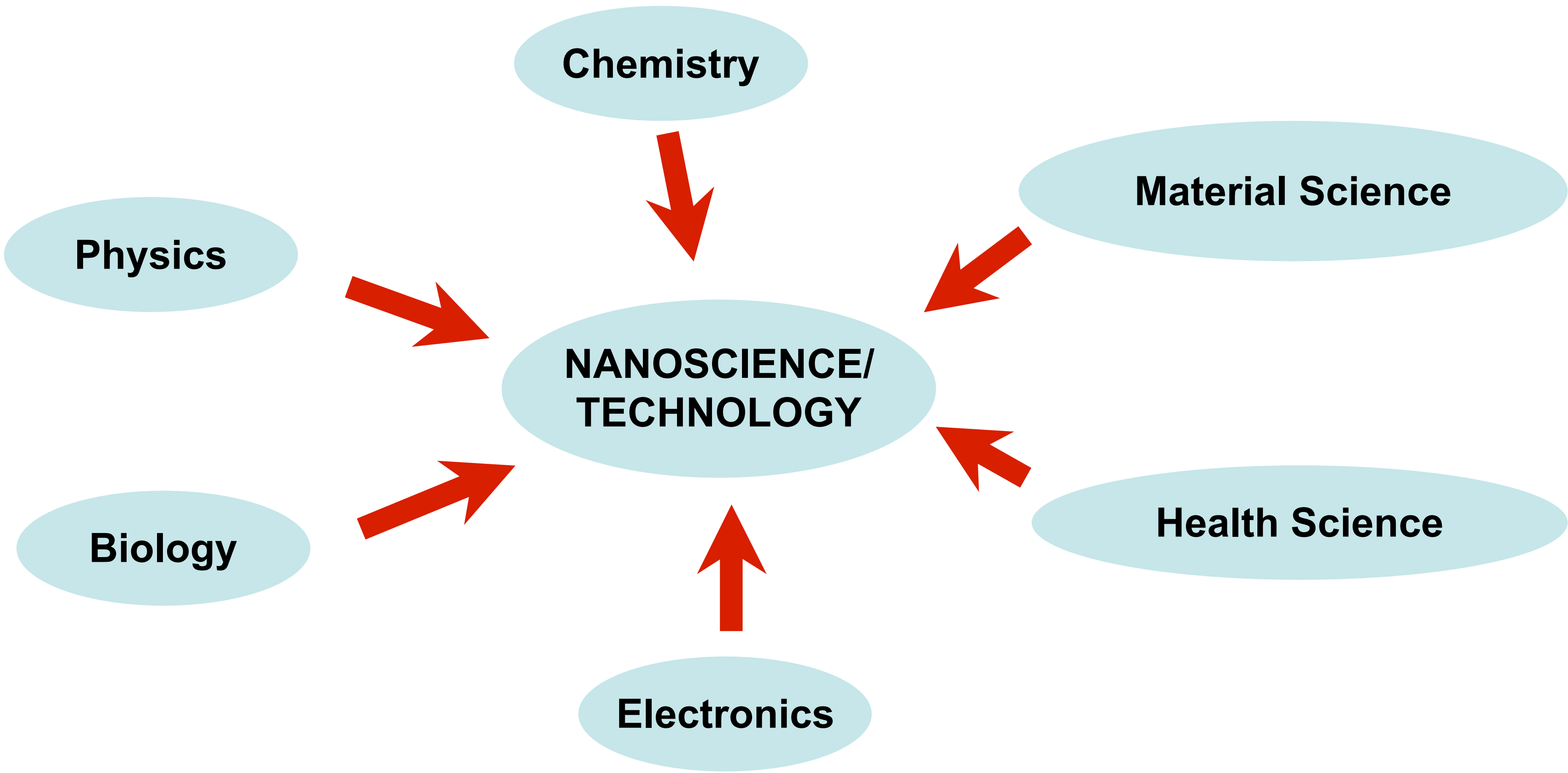
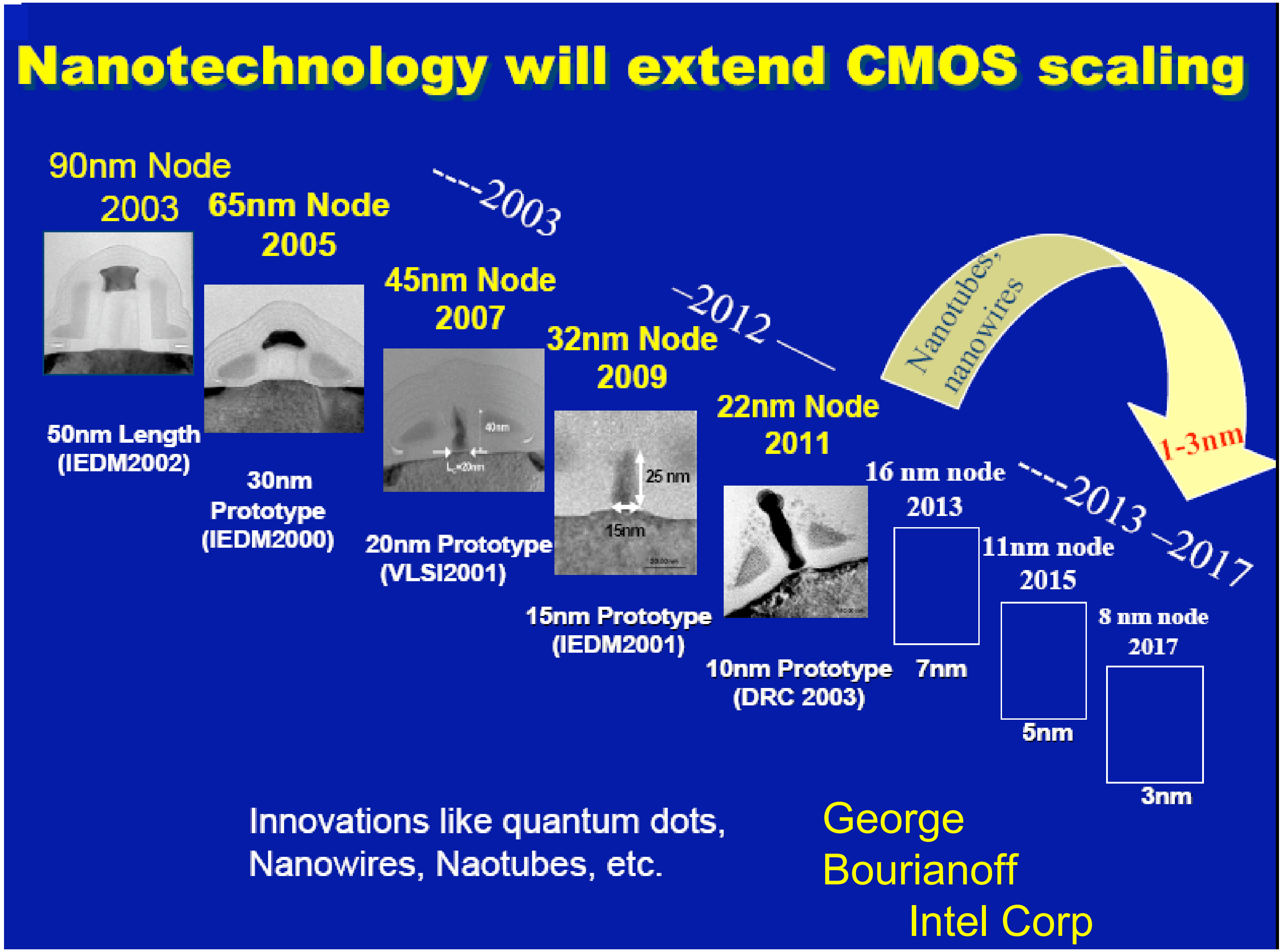
Outline

- Nanoscience crossing disciplines
  - computational nanoscience
    - characteristics
    - challenges/opportunities
- Software development
  - Needs for nanoscience
  - User types
  - Proprietary versus free software

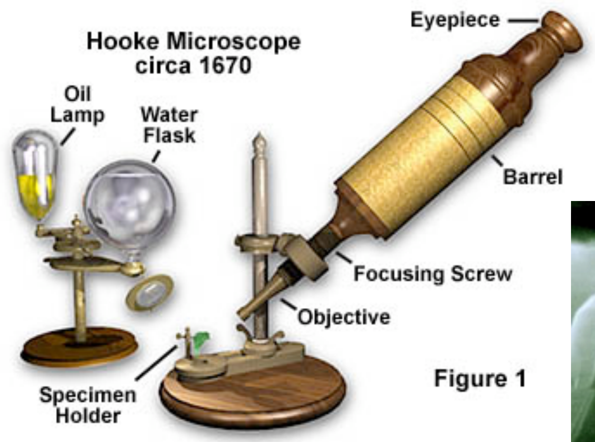
Nanoscience/technology is Truly Cross Disciplinary



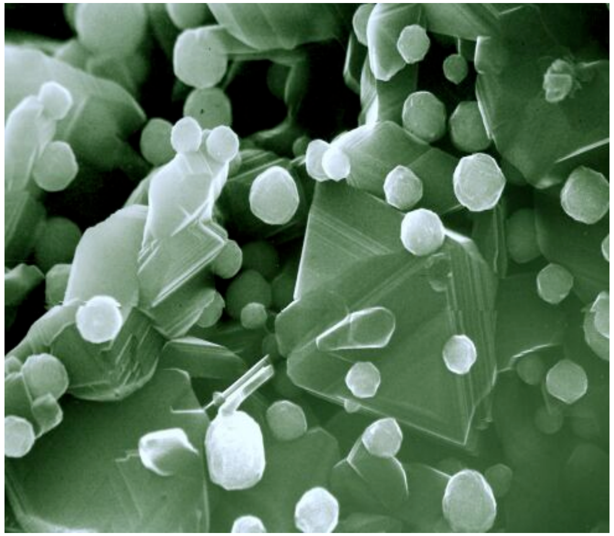
Nanoelectronics on its way: Intel Roadmap



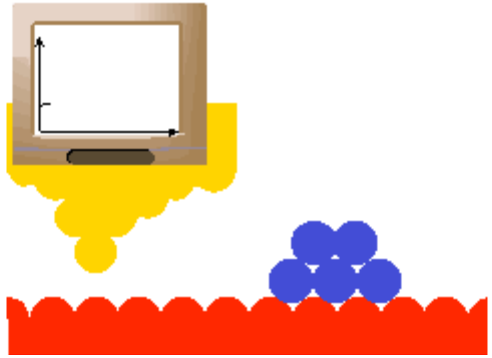
Enabling Nanotechnology



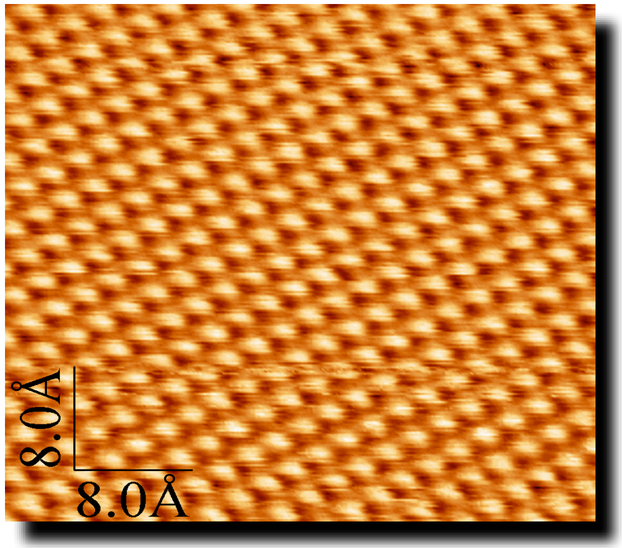
Optical magnification
mm → μm (→250 nm)



SEM:
Scanning Electron Microscopy:
Detects backscattered electrons
mm → μm (→ nm)
500nm particles on porous substrate

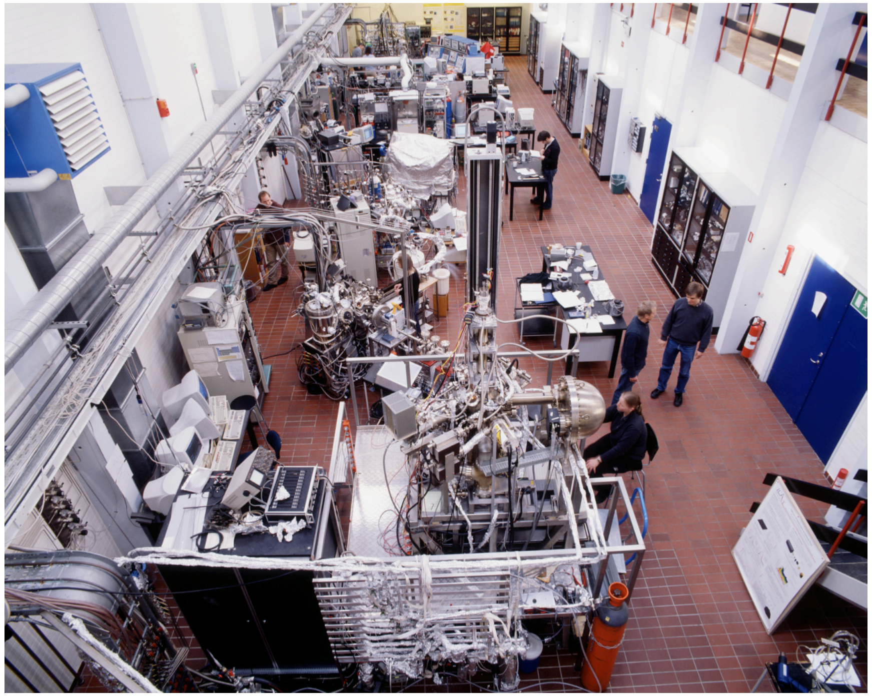


STM:
Scanning tunnel microscopy
atomic resolution



8 nm x 8 nm

Nanoscience Facilities



Supercomputing
(Quantum) simulation tools

Nanoscale synthesis and
characterisation facilities

Computing is essential in nanoscience/technology!

”Ab initio” Nanoscientific Computing

- Long tradition in physics and chemistry
- In principle we know what to compute
- Approach towards ”ab initio” description of the electronic structure problem
  - Configuration Interaction
  - Quantum Monte Carlo
  - ..
  - Density-Functional Theory
  - ..
  - Interatomic potentials
  - United-atom force fields
- Often predictive power
- Very computer intensive!

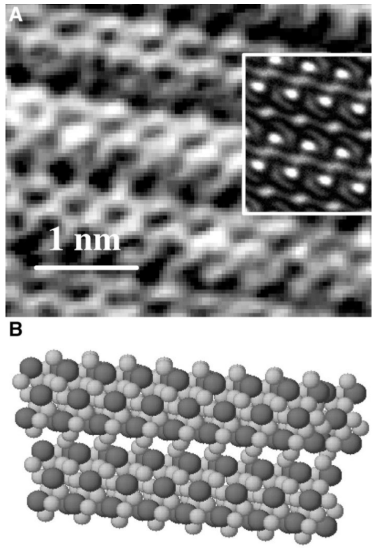
↑ Accuracy

↓ Speed

Computing: An Essential Nanoscience Tool

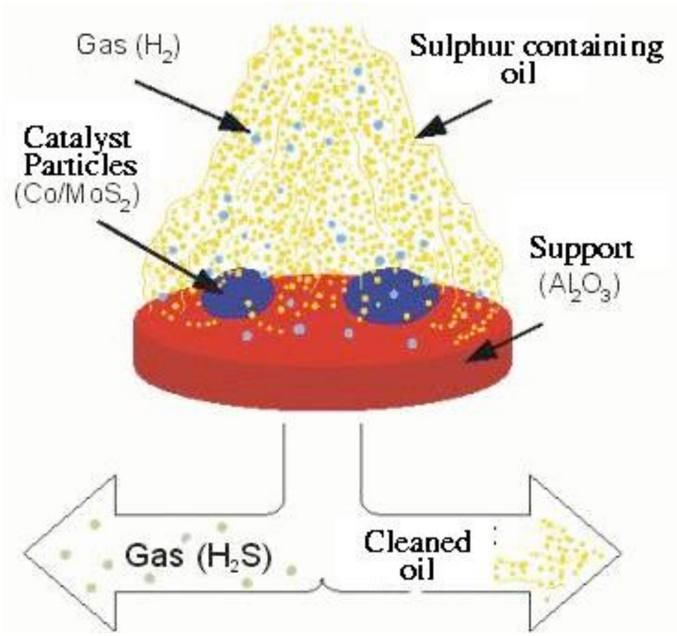
MoS_2 – a remarkable material

Layered structure – nanotube formation



Remskar et al., *Science* **292**, 479 (2001)

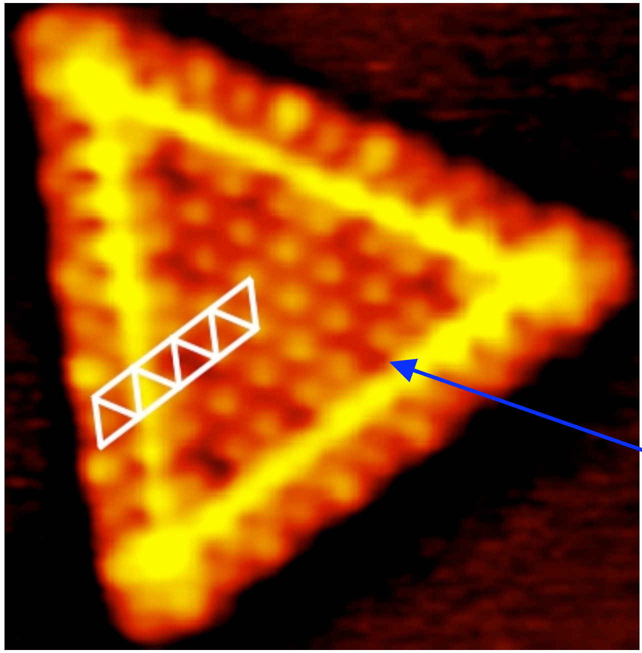
Lubricant



Catalyst for hydrodesulfurization (HDS)

MoS2 Nanostructures

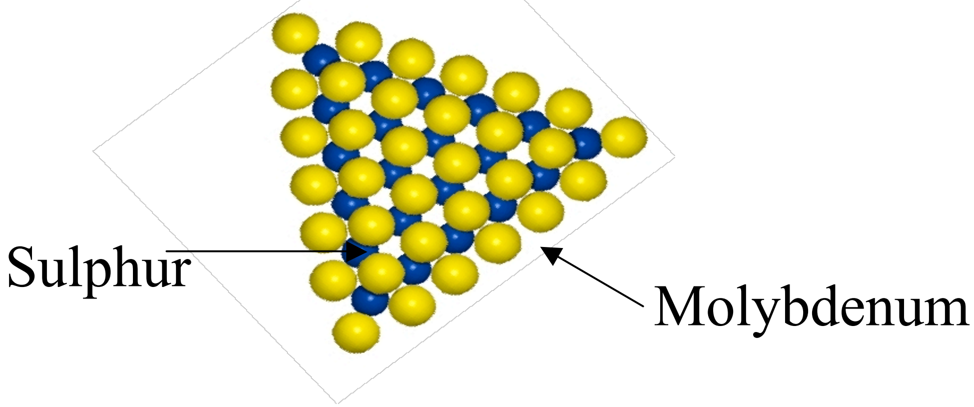
Helveg et al., PRL 84, 951 (2000)

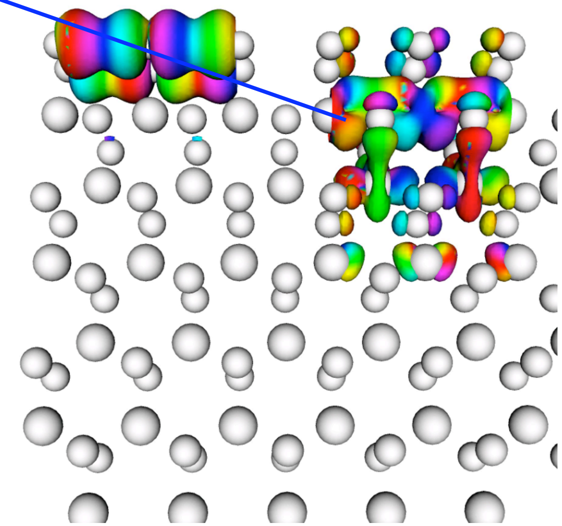


Scanning Tunneling Microscopy experiments on MoS_2

Bollinger, Lauritsen, Jacobsen, Nørskov, Helveg, Besenbacher, *PRL* **87**, 197803 (2001)
Bollinger, Jacobsen, Nørskov, *PRB*

Edges believed to be "active sites" for HDS

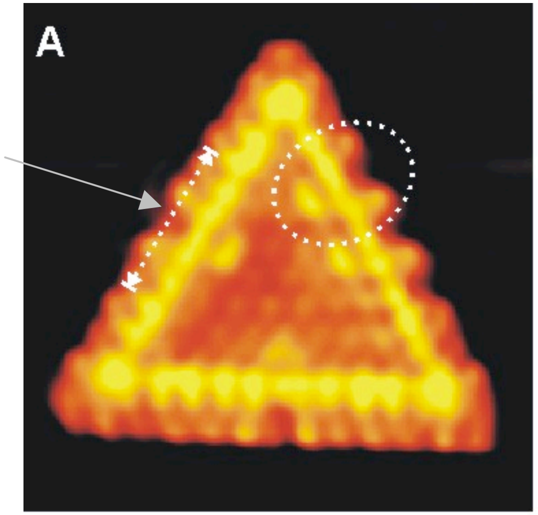


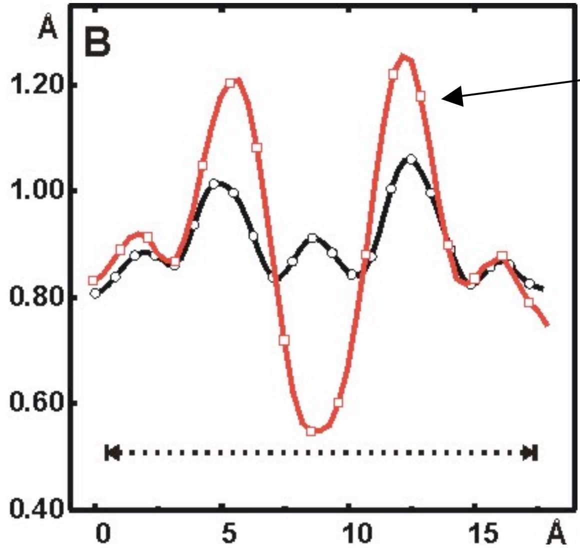


DFT calculations reveal conducting edge states

Thiophene Chemistry of Edge State

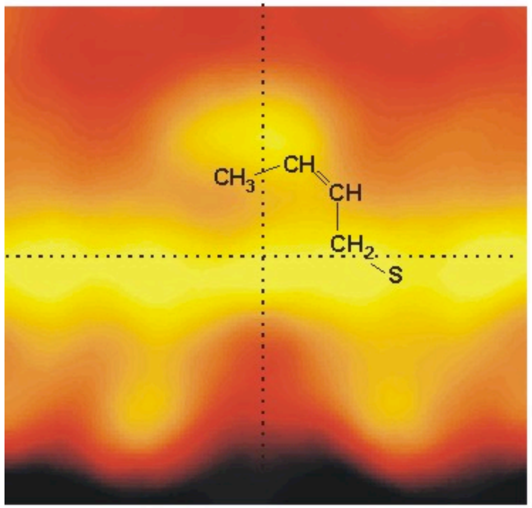
Line scan

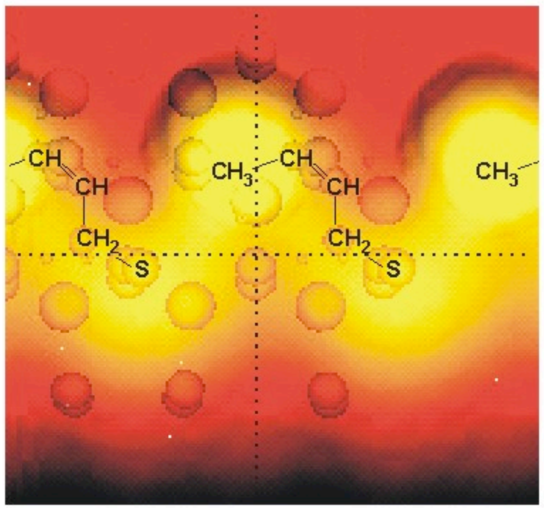




Thiophene chemisorbed (after predosing with hydrogen!)

Measured STM image

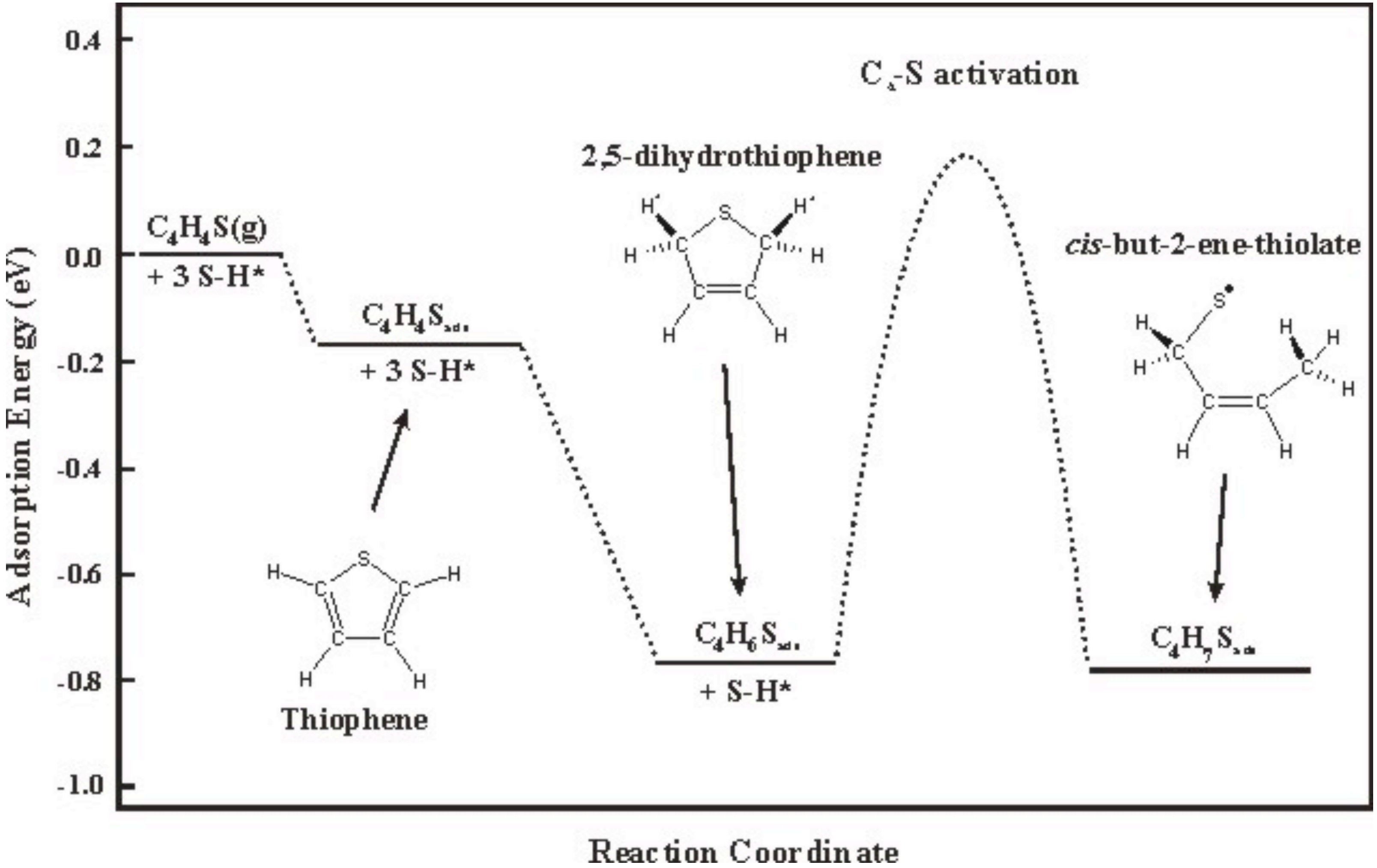




Simulated STM image

Lauritsen et al. Nanotechnology 14, 385 (2003)

The Hydrogenation Path



Lauritsen et al. Nanotechnology 14, 385 (2003).

”BRIM” technology

(Haldor Topsøe A/S)

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Haldor Topsoe > News > **Topsoe extends their family of BRIM™ hydroprocessing catalysts**

Topsoe extends their family of BRIM™ hydroprocessing catalysts
New hydrocracker pre-treatment and ULSD NiMo catalysts

Lyngby, 12 January 2006

The low-sulphur fuel market continuously calls for improved hydrotreating catalysts. In order to fulfil this need, Topsoe has developed a new catalyst preparation technology, giving highly active hydroprocessing catalysts. This new proprietary BRIM™ technology not only optimises the brim site hydrogenation functionality, but also increases the Type II activity sites for direct desulphurisation. The first two commercial catalysts based on the brim technology were Topsoe's TK-558 BRIM™ (CoMo) and TK-559 BRIM™ (NiMo) for FCC pre-treatment service. This was in 2004 followed by a new CoMo catalyst, TK-576 BRIM™, for ULSD production.

Since then, Topsoe has sold BRIM™ catalysts to more than 50 hydrotreating units.

Topsoe has now introduced two new NiMo products based on the BRIM™ technology:

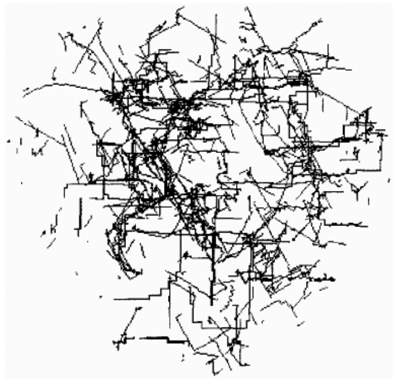
Some Challenges

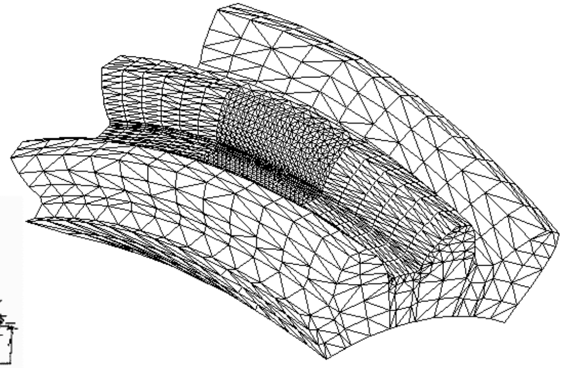
- Increased accuracy and speed
  - Density-Functional-Theory level:
    - Better description of van der Waals systems (biosystems, water,...)
    - Exchange and correlation of oxides/carbides
    - Excited states and dynamics
- The scale problems
  - Space
  - Time
  - Separation of relevant space (and time) scales?

The Nano-Macro Connection

Scale problem in space and time.

Dislocation dynamics



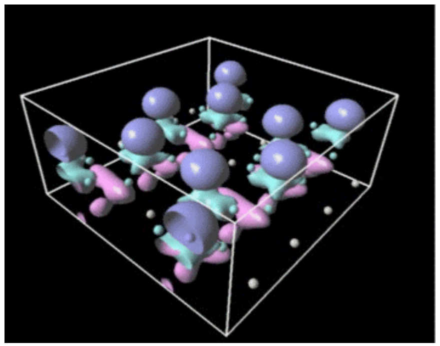


Finite element

Molecular dynamics

Quantum mechanics

Materials length scales

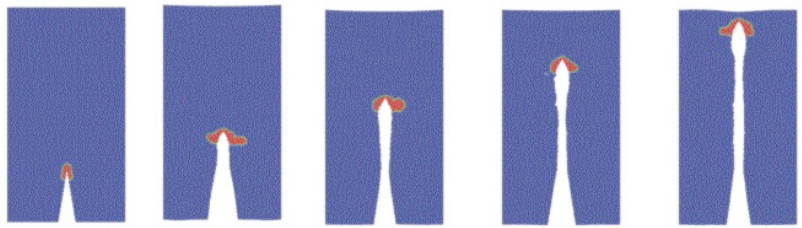


Density Functional Theory
- General applicability to atomic/electronic systems
- Compute intensive

Center for Atomic-scale Materials Physics
Center for Nanotechnology at DTU

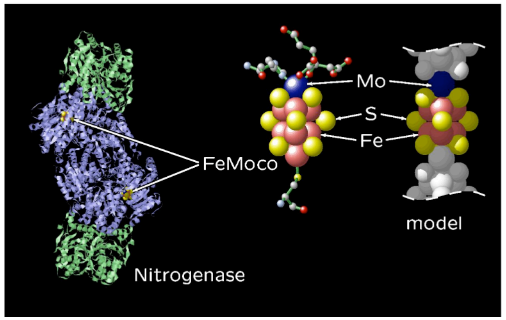
Multiscale Modeling

Cracking of Si:



http://www.wag.caltech.edu/home/mbuehler/cmdf/

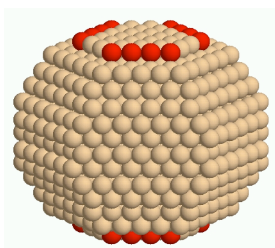
Ammonia production by Nitrogenase:



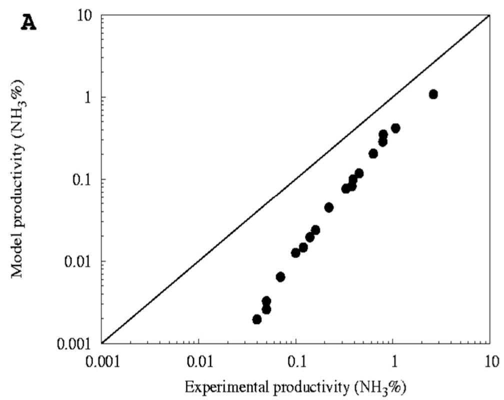
Multiscale modelling (QMMM) necessary to describe full enzyme.

B. Hinnemann and J. K. Nørskov, J. Am. Chem. Soc. **126**, 3920 (2004).

Production of ammonia by Ruthenium catalyst:



Reaction kinetics →



Honkala et al., Science (2005).

CAMP Center for Atomic-scale Materials Physics
Nano•DTU Center for Nanotechnology at DTU

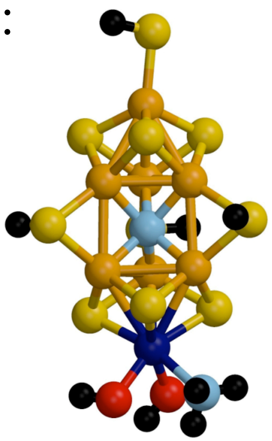
Nano-Macro Connection: Identifying Descriptors

Example: Bio-inspired hydrogen production

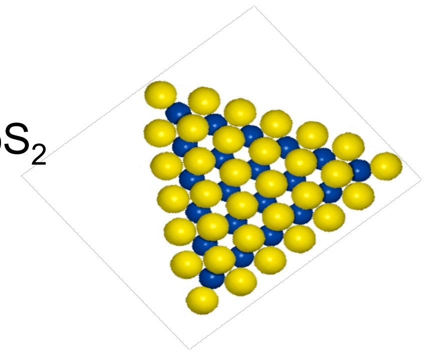
Descriptor: Hydrogen bond strength to electrode material

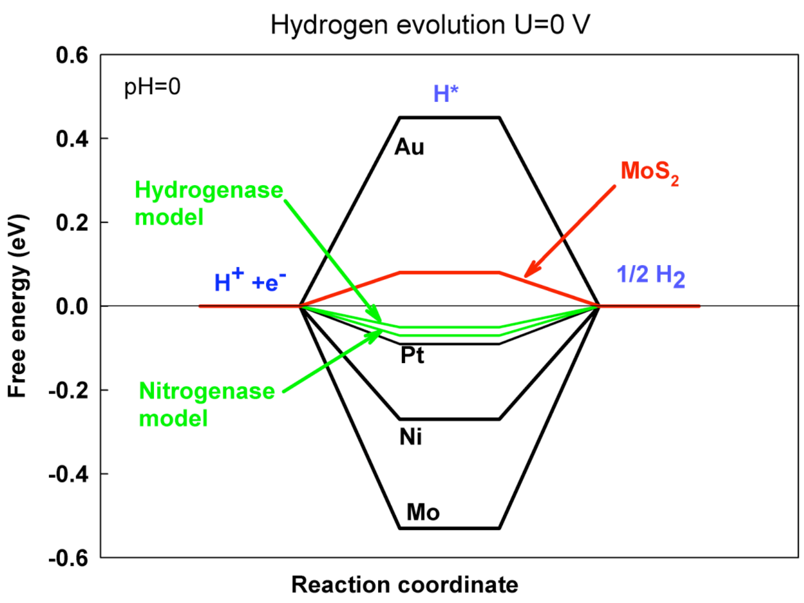
Nitrogenase: Can split hydrogen!

Cluster of Mo, Fe, S



MoS_2





Pt or Pt alloy
the usual electrode

Experimentally confirmed hydrogen production by MoS_2

Hinnemann et al. JACS (2005)

Nano-Macro Connection: Identifying Descriptors

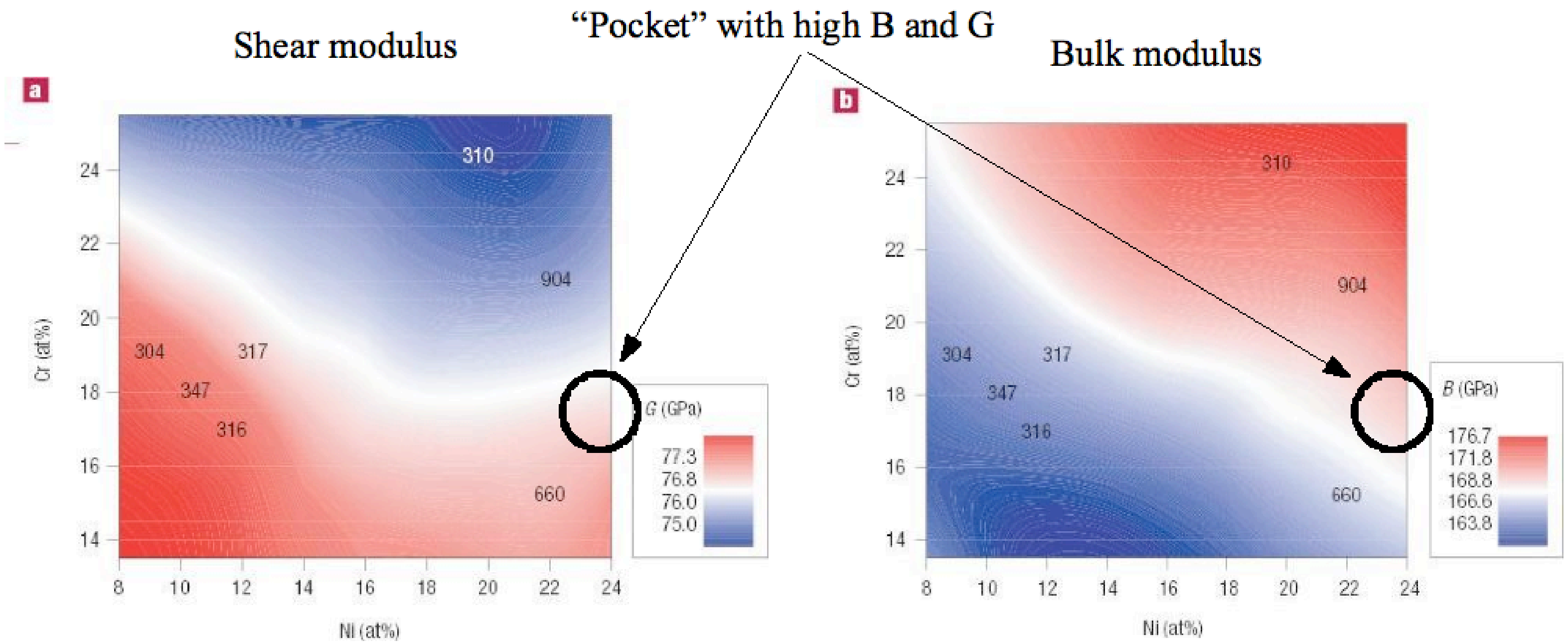
Example: Stainless steel optimization: Fe-Cr-Ni

Cr provides corrosion resistance
Ni stabilizes austenite (fcc) phase

EMTO basis
Coherent Potential Appr.

Descriptors:

Shear modulus G ~ hardness
Bulk modulus B ~ cohesion ~ opposition to rupture
B/G ~ ductility



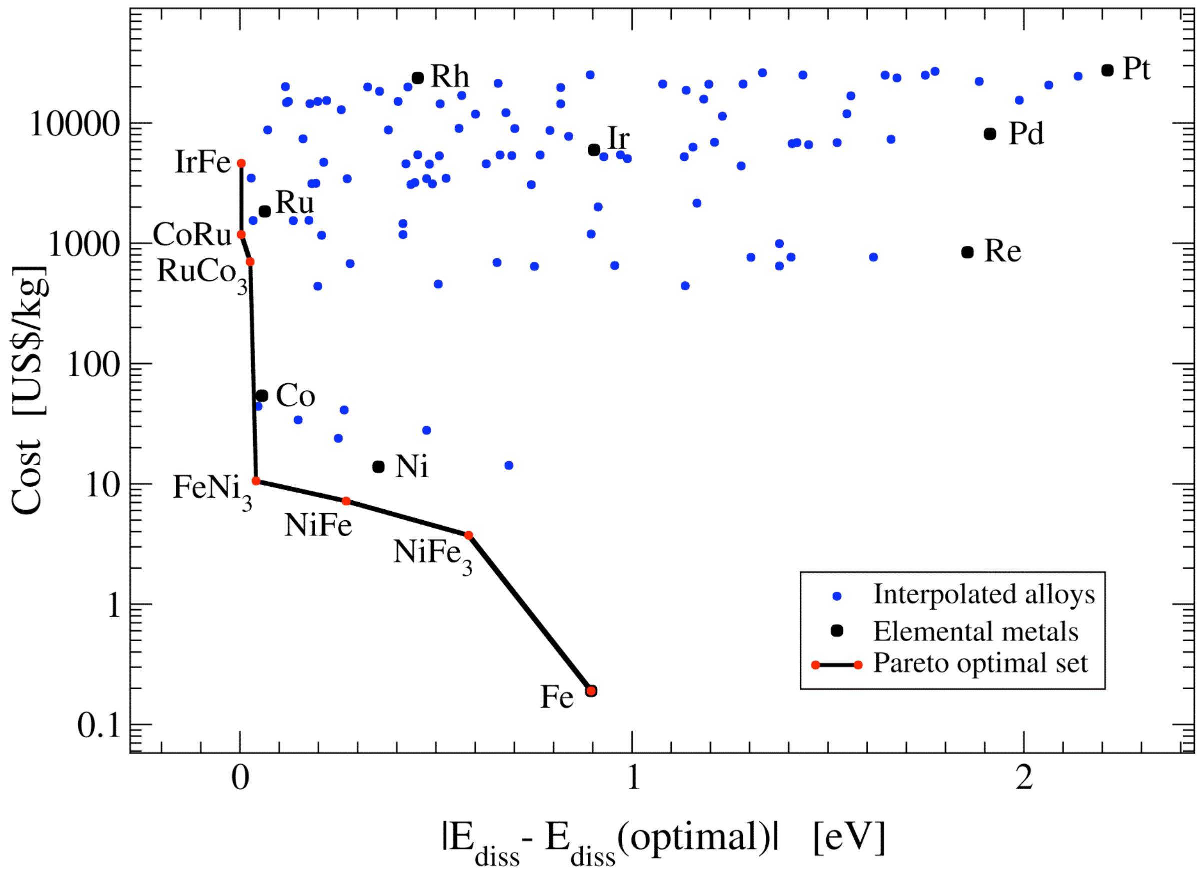
Vitos, Korzhavyi, Johansson, Nature Materials **2**, 25 (2003)

Towards Comp. Nanodesign: Search for Methanation Catalyst

A_xB_{1-x} alloys, where x=0,0.25,0.5,0.75,1, A,B=Ni,Pd,Pt,Co,Rh,Ir,Fe,Ru,Re

$CO+3H_2 \rightarrow CH_4+H_2O$

Descriptor:
Optimal value for oxygen dissociation energy



Andersson, Bligaard, Kustov, Greeley, Johannessen, Larsen, Christensen, Nørskov (2005)

Software Needs for Nanoscience

- Software to perform well-defined tasks
  - Energy, forces
  - Atomic motion
    - Structural optimizations, determination of transition states
    - Molecular dynamics
  - Excitation spectrum
    - electronic dynamics
  - Materials screening
    - Search algorithms
- Users want
  - Reliability
  - High speed - low memory
  - Flexibility - many ”features”

Different Users

- Unexperienced/occasional user
  - Help to setup and get going with simple tasks
    - Graphical interface
  - Extensive checking for mistakes/misuse
- Power user/researcher
  - Perform complicated tasks
    - Scripting
  - New unexpected use of code
  - At-the-edge performance
  - Code development
    - Well-structured, ”layered” source code to dig into
    - Easy to try out new ideas - fast prototyping
    - Easy bug tracking

Trends in Software Development

- Increasingly advanced codes - hard to do for one person - many international collaborations
- Better use of tools
  - Code repositories (cvs, svn), multiuser development, tagging, branching
  - Developer communication (mailing lists, wikis,...)
  - Automatic code checking (test suites) and generation of documentation
  - Extensive use of optimized libraries (FFTW, BLAS,...)
- Different programming languages (speed, structure, scripting...)
- Towards standards for file formats
- Competition between proprietary and free software

Proprietary versus Free Software

Gaussian.com THE OFFICIAL GAUSSIAN 03 WEB SITE

VASP Vienna Ab-initio Simulation Package

atomistix

CASTEP

CHARMM

siesta

FS atom

abinit.org

CAMP Center for Atomic-scale Materials Physics ASE

www.gromacs.org

MIKA (CSC)

MMTK

OCTOPUS

CP2K

PWscf Plane-Wave Self-Consistent Field "The computer is a tool for clear thinking" Freeman J. Dyson

and many more ...

Proprietary versus Free Software

- Unexperienced/occasional user
  - Nice and easy user interfaces with some commercial codes
- Power user/researcher
  - Hard to do everything alone
  - Source code access
  - Right to modify and redistribute source code
  - Participate in code planning/strategy

- Survival of the fittest?
- Funding of code development?