Multiscale Materials Modelling with High Performance Architectures

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CAPACITIES

e-infrastructure

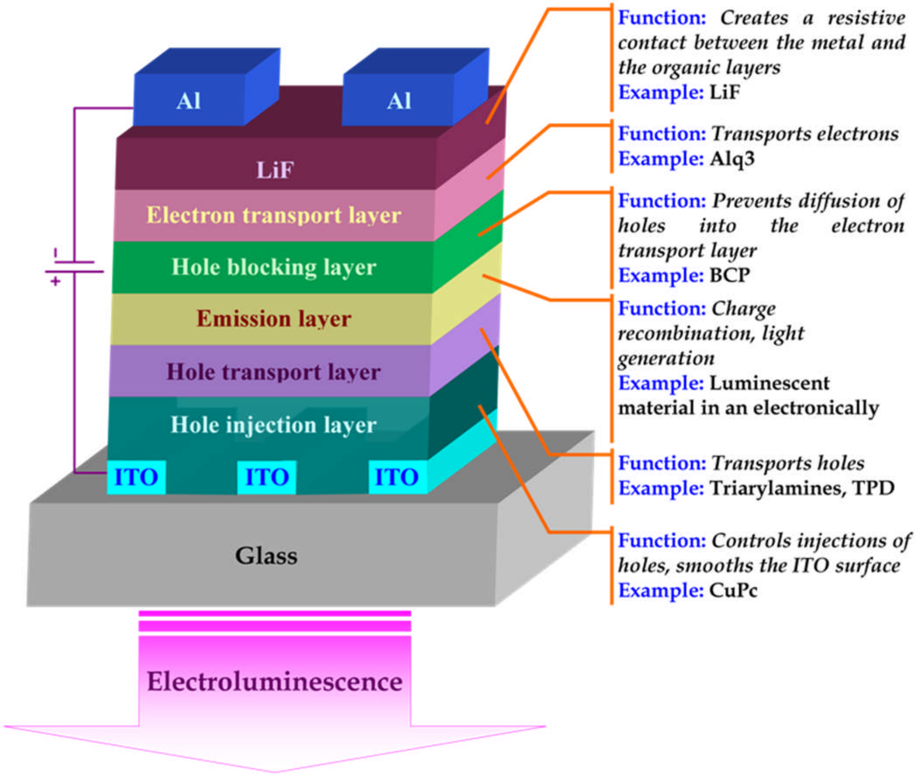
The project MMM@HPC is funded by the 7th Framework Programme of the European Commission within the Research Infrastructures with grant agreement number RI-261594.

Outline

- From frustration to ideas
  - Multiscale modeling of electronic transport through amorphous thin films
  - Atomic Transistor
- From ideas to solutions
  - What is MMM@HPC ?
  - How can I use it (tomorrow) as a scientist to accelerate my research?
- From solutions to results:
  - Polymer Sorting by Carbon Nanotubes
  - Magnetic Storage using Graphene Flakes
  - Electronic Transport through amorphous organic films

Multiscale Modelling Example

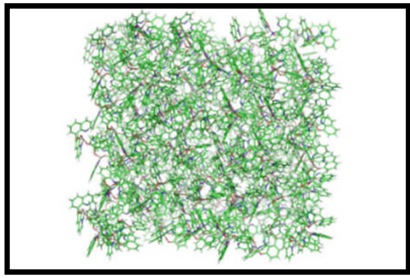
- Multiscale Modelling techniques for amorphous thin film materials
- Efficiency and durability can be improved
- Challenge: understand conductance and aging properties (at the molecular level)
- Goal: simulate growth of thin organic films & interfaces properties and properties



Schematic illustration of multi layer structure of small molecule based OLED

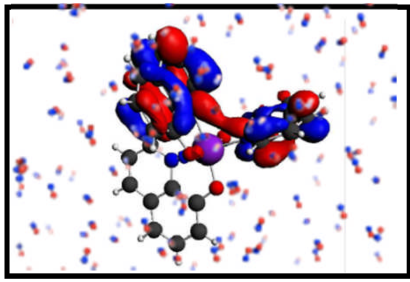
Multiscale Simulation Steps: Mobility Calculation

STEP 1



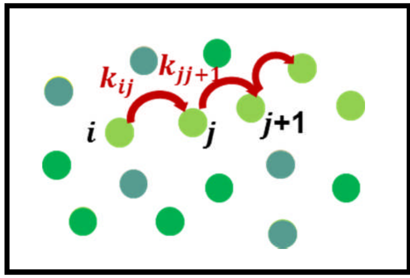
MORPHOLOGY

STEP 2



LOCAL ELECTRONIC STRUCTURE

STEP 3

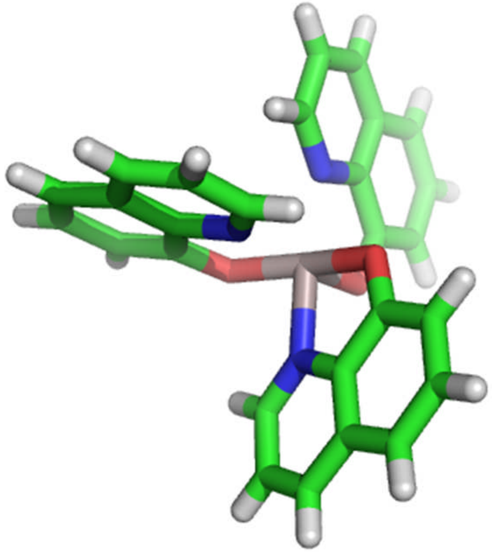


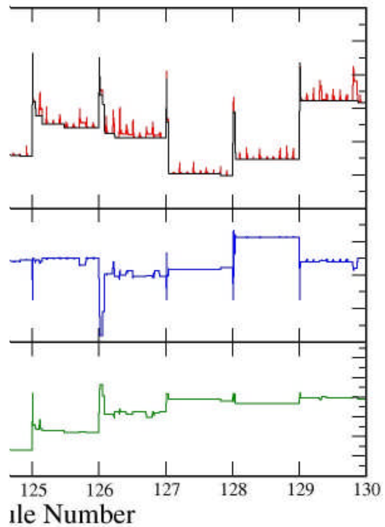
CHARGE TRANSPORT

MACROSCOPIC PROPERTIES

Growth of amorphous organic films

MMM @HPC



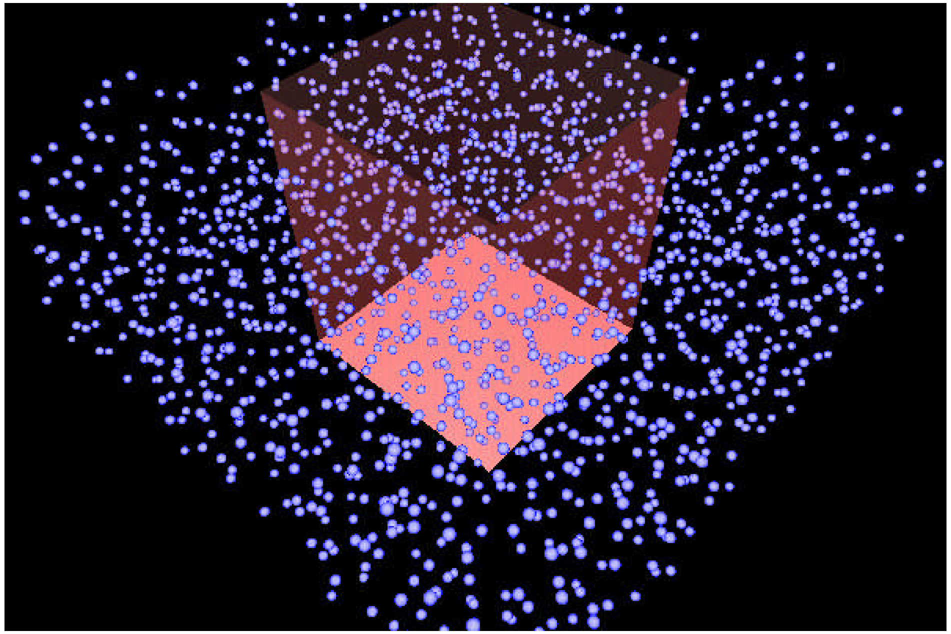


DEPOSIT: Individual molecules are deposited, search for an optimal position and incorporated into the film

Linear Scaling Approach → (D. Danilov)

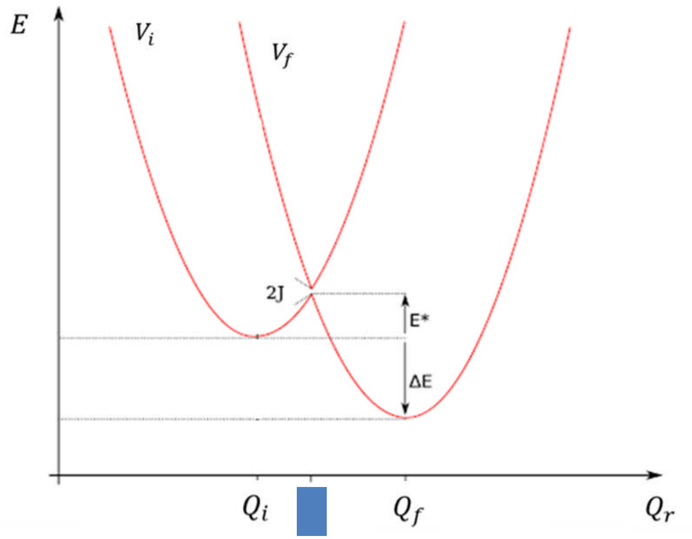
Realistic Morphologies .....

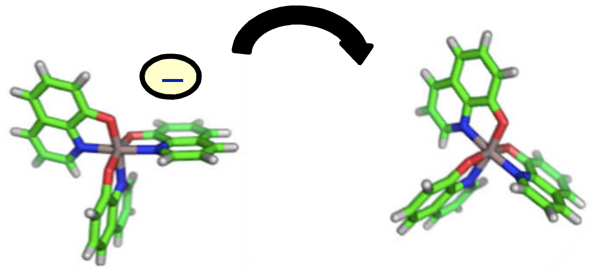
- DEPOSIT: deposition of individual molecules on preformed layers
- MC protocols with O(N) scaling
- 1000 molecules ~ 2-3 hours
- Sample size:
  5-50 nm x 20 nm x 20 nm
- Analysis of conduction pathways (percolation problem)
- Interfaces, stacks, I/O interfaces ....



Electronic Structure: Hopping Rates

- Estimating Marcus' hopping rate with (DFT) Turbomole or semiempirical methods (MOPAC)





$$\Gamma_{if} = \frac{2\pi}{\hbar} |J_{if}|^2 \frac{1}{(4\pi\lambda k_B T)^{1/2}} \exp\left(-\frac{(\lambda + \Delta E)^2}{4\lambda k_B T}\right)$$

R. A. Marcus, Rev. Mod. Phys. **65**, 599 (1993)

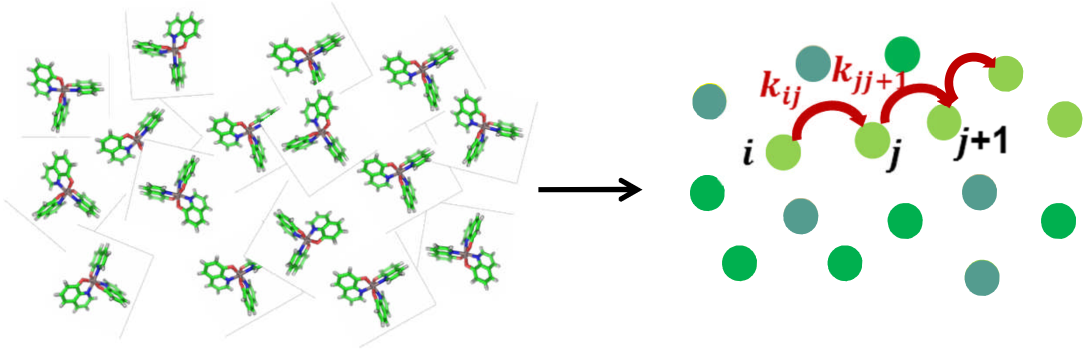
- J_{if} of a molecular dimer:

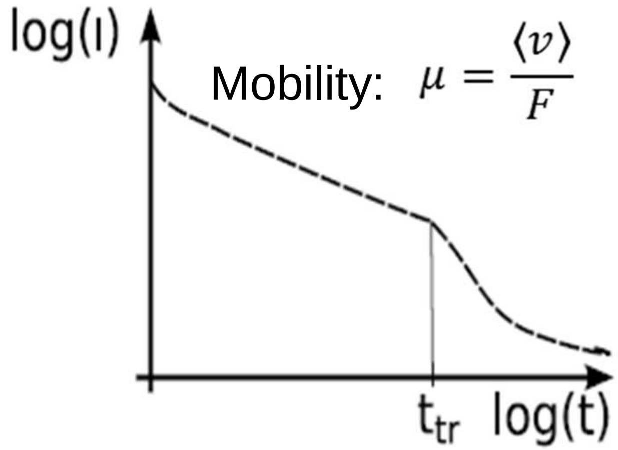
$$J_{if} \approx < \Phi_i^M | H_{KS}^D | \Phi_f^M >$$

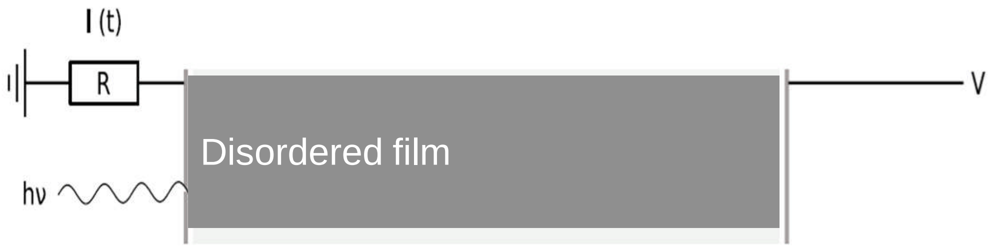
- Or:

$$J_{if} \approx \frac{H_{if} - \frac{1}{2}(H_{ii} + H_{ff}) S_{if}}{1 - S_{if}^2}$$

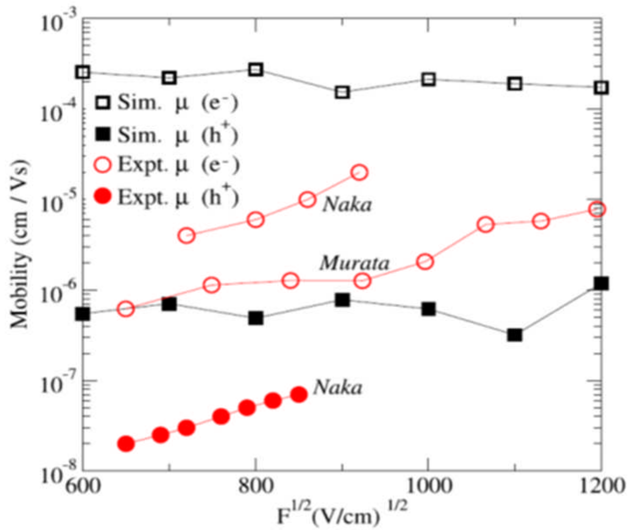
Charge Transport: Kinetic Monte Carlo





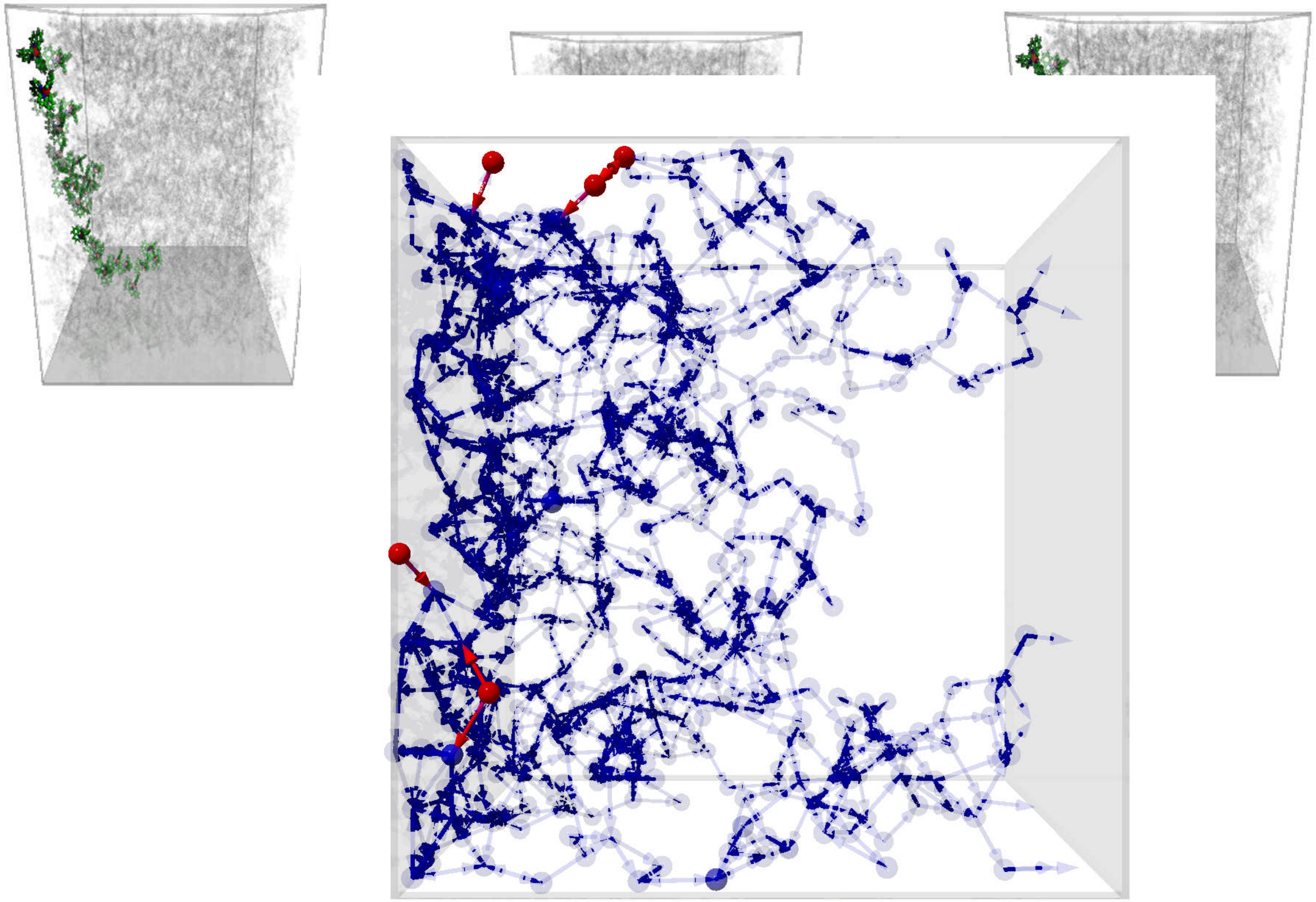


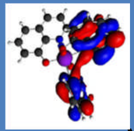
$$\frac{\mu_e}{\mu_h} \approx 10^2$$



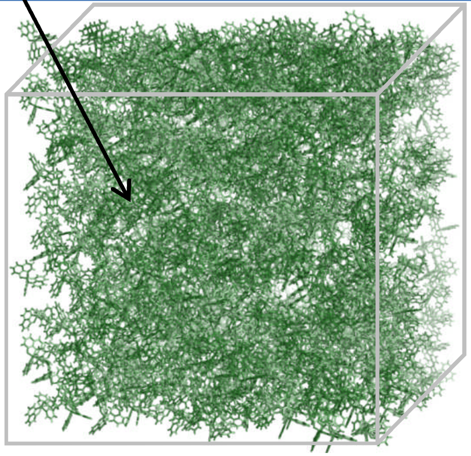
J. J. Kwiatkowski, *et al*, PCCP **10** 1852 (2008)

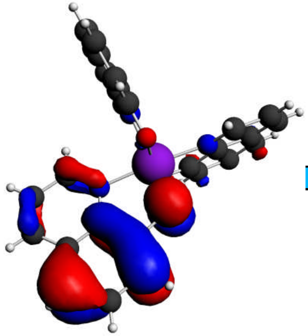
Individual Paths and Clusters

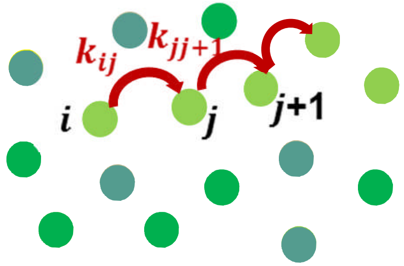


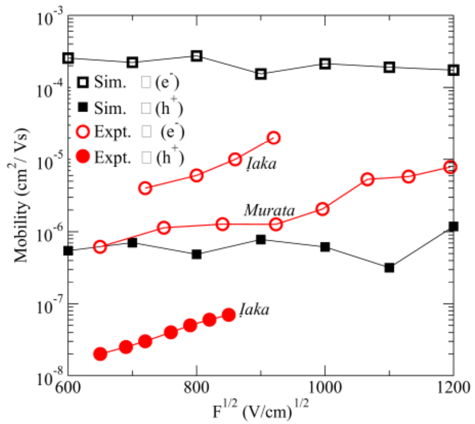


Multi-Scale-Simulation Logisitics









- Involved 4 groups
- Data transferred from one group to the next
- Data conversions
- Reproducibility

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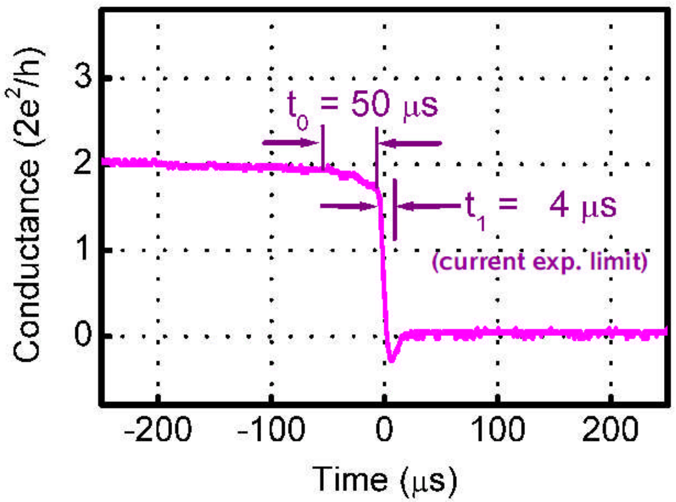
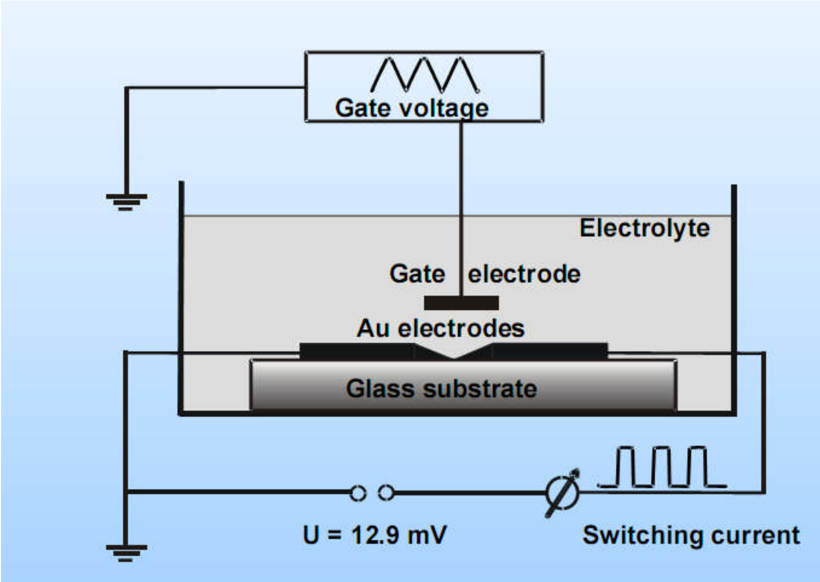
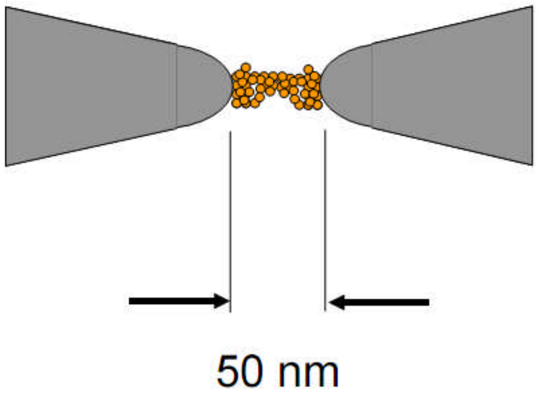
Gate Controlled Current Switching

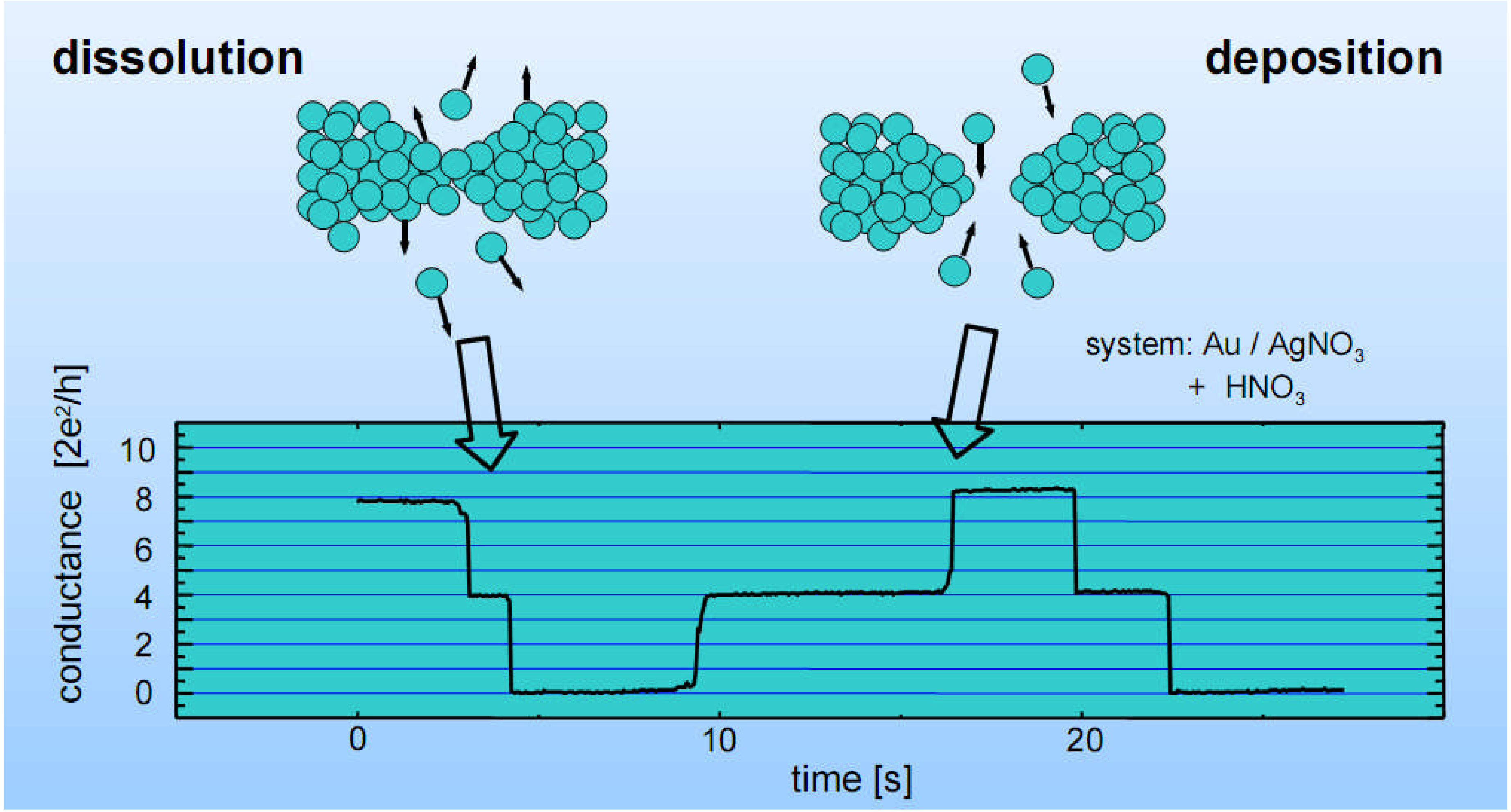




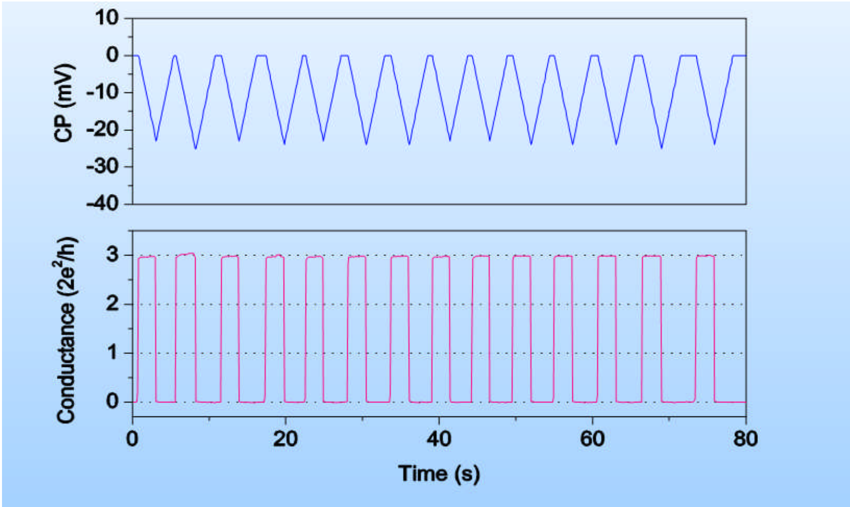
Small changes in the gate voltage induce reproducible on/off jumps in the current

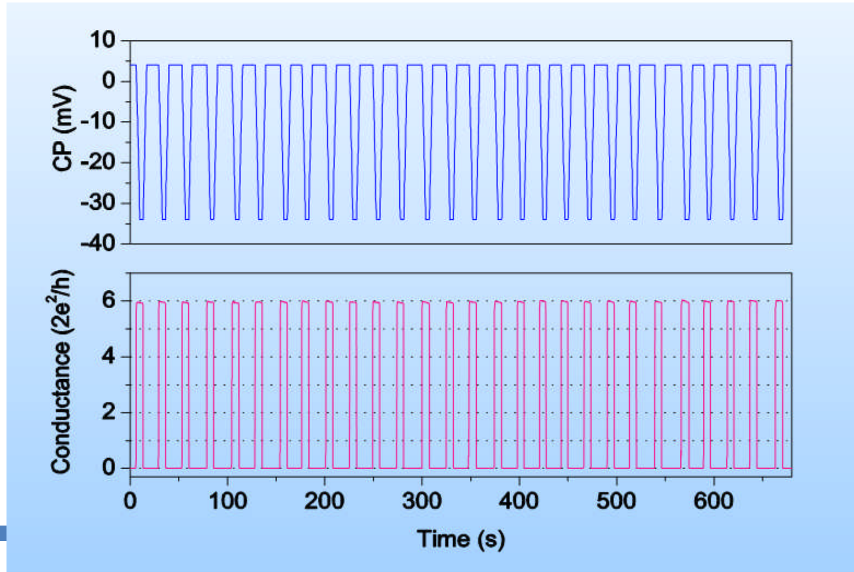


Switching Conductance on the quantum scale



Tunable quantized conductivity

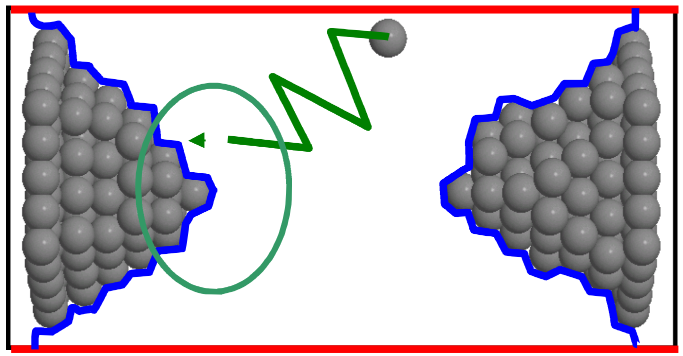


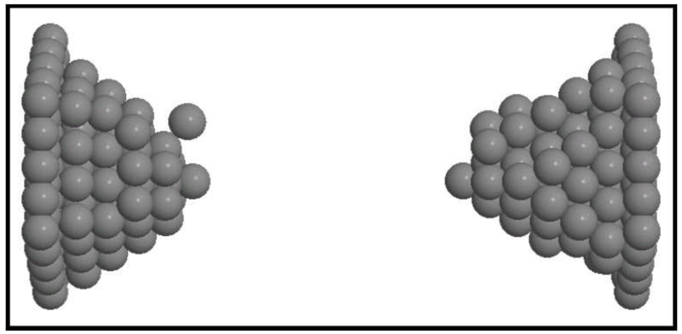


- Variation of the control loop in switch construction permits selection of desired contuctivity levels
- We observe levels from N=1 to N=20 for Ag contacts

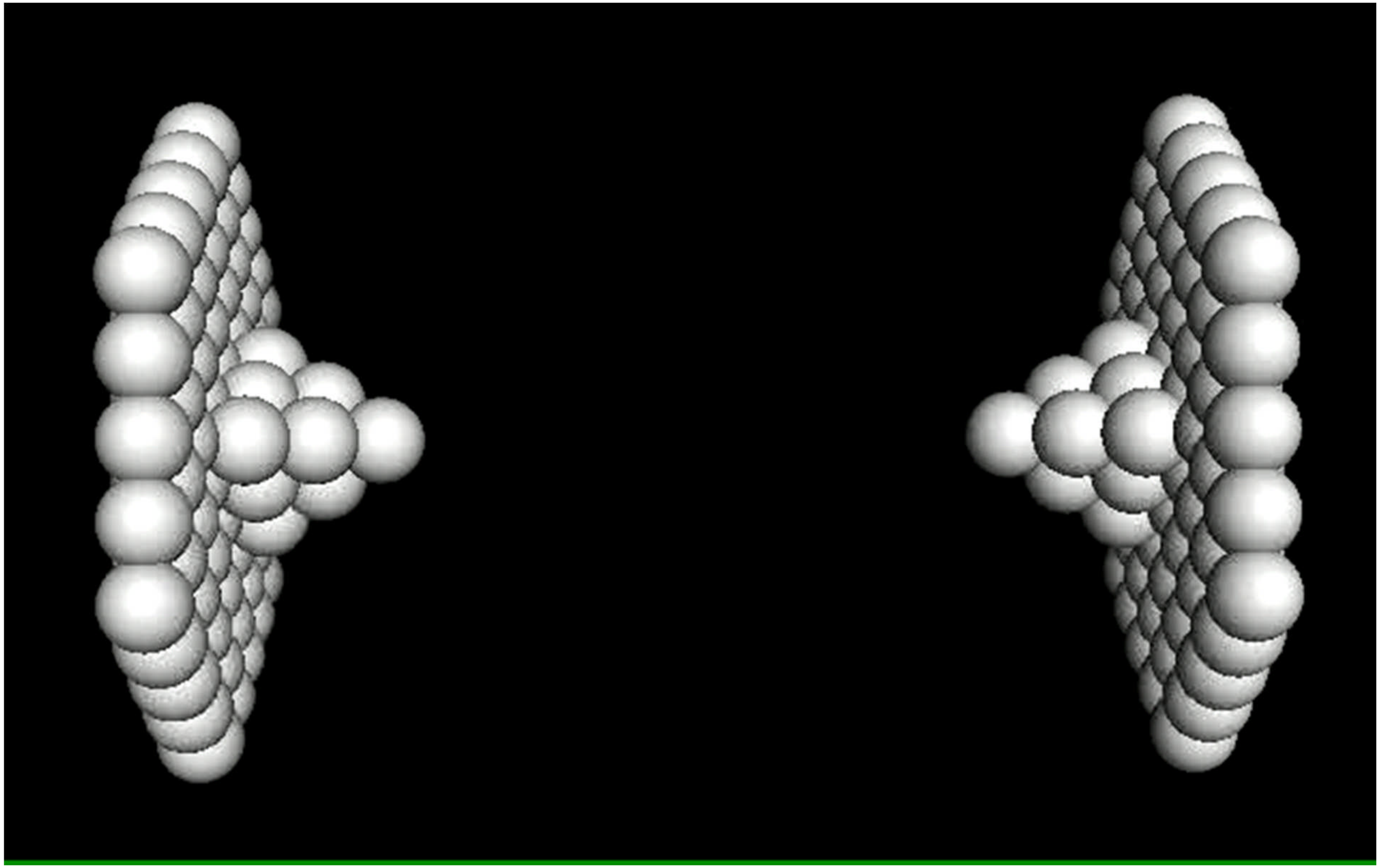
Modelling of Deposition and Switching

- Deposition of individual atoms by stochastic simulation
  - Classical material-specific potential (Gupta)
  - Coulomb Potential (Poisson equation)
  - electrochemical Potential
- Relaxation of the surface in a defined region
- 1000s of simulations possible
- Computation of conductance
- Modelling of the switching process

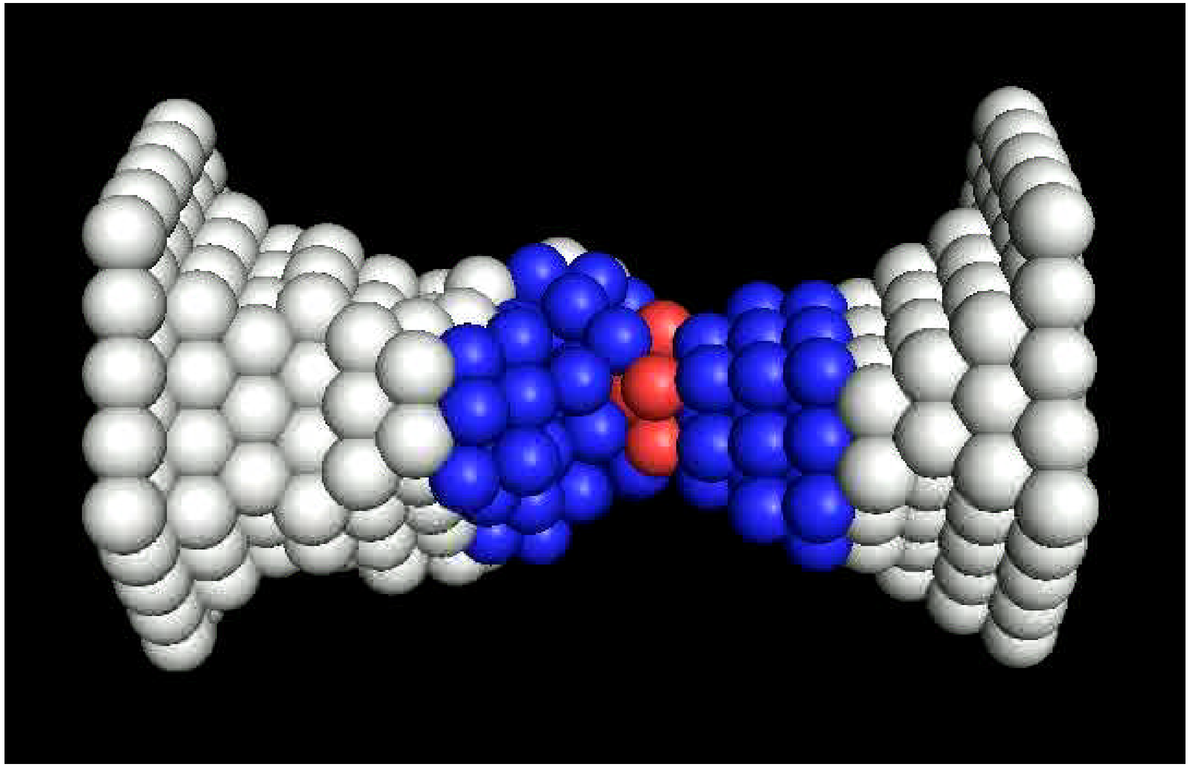




Single Atom Transistor

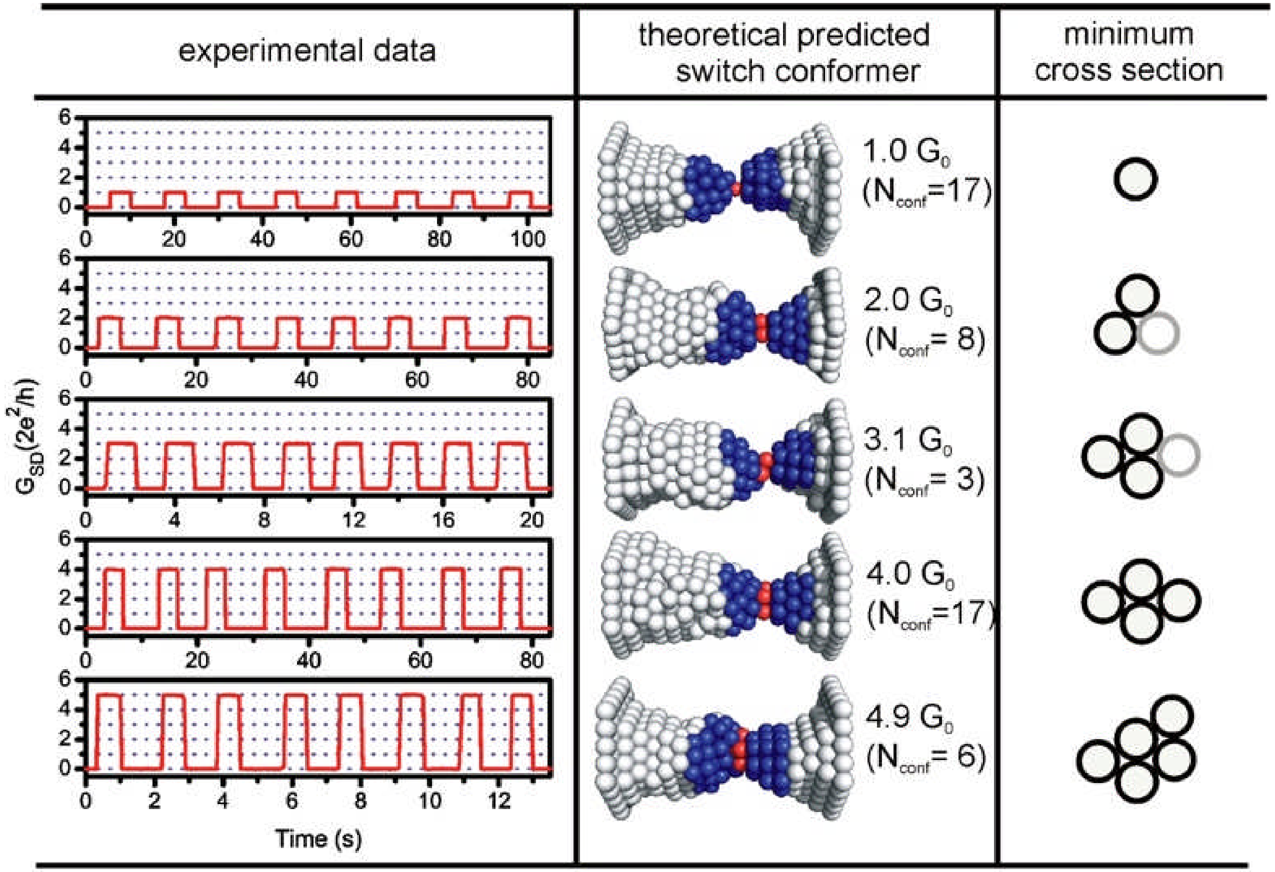


Bistable Electrode Reconstruction



Switchable Conductivity

MMM@HPC



- MM: Growth and Switching in Single Atom Transistor
- QM: Transport Landauer formalism
- O(N) Method: Recursive Green-function approach
- Continuum Model for Electrolyte
- Mechanism: Bistable Electrode Reconstruction

Nano Letters **8,** 4493 (2008)

Adv. Mater. **22**, 2033 (2010); Appl. Phys. Lett. **100**, 203511 (2012)

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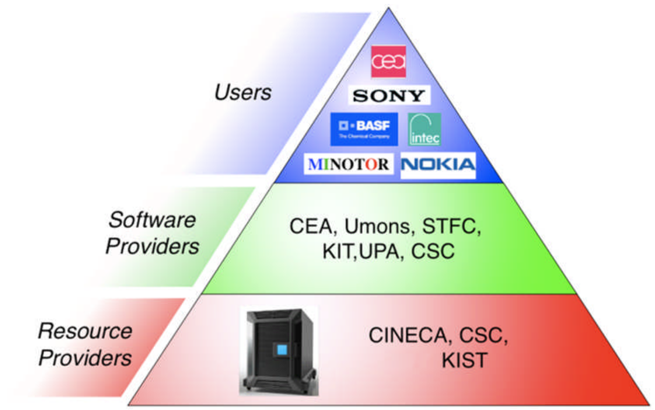
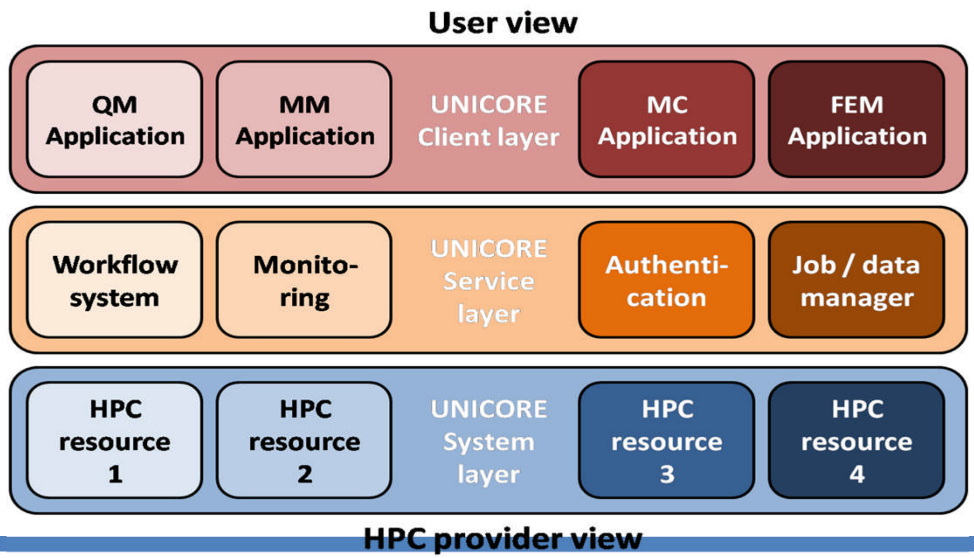
Concept

- MMM@HPC integrates competence of
  - HPC providers,
  - Software providers
  - Software users (including industry)
- Provision of a toolbox of simulation tools that can be combined in many different application workflows
- Adaptable, reusable and extendable interfaces & workflows





Implementation

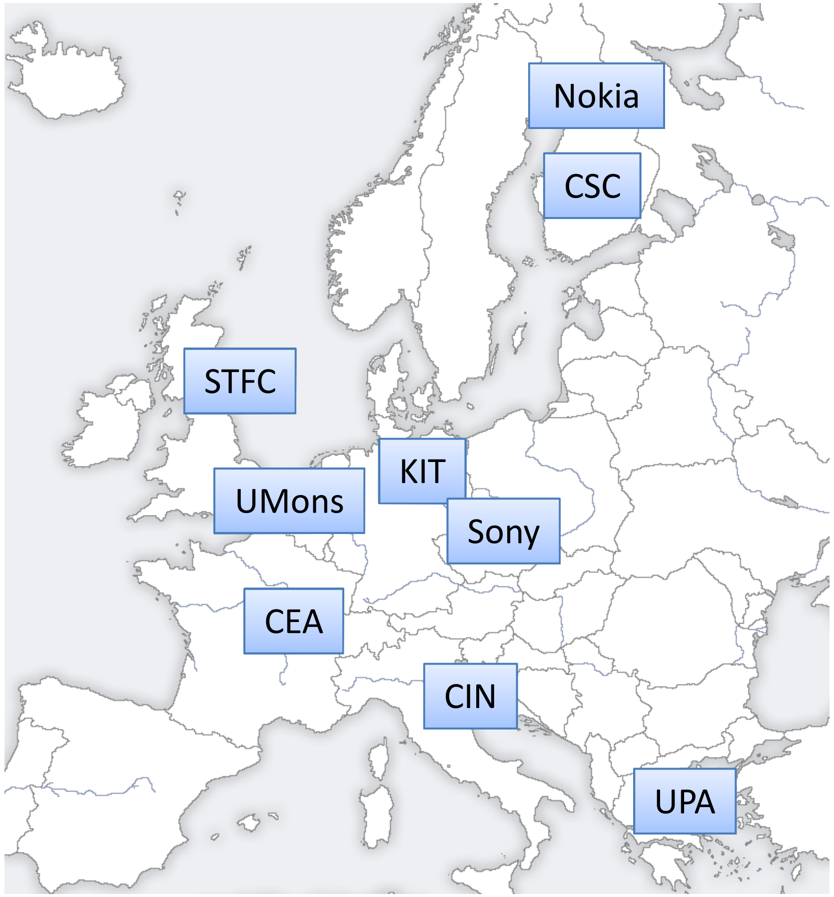
- Implements workflow components as services using Unicore/Gridbeans
- Deployed productively in DEISA/PRACE infrastructure

MMM@HPC Implementation

- **open & extendable concept**
  - diverse, growing and evolving user community
  - modular
  - maintainable and adaptable to novel hardware platforms
  - secure
- **high priority applications in the European research agenda**
  - Energy conversion (OLED)
  - Energy storage (Li-Ion Batteries)
  - Energy transport (molecular & carbon based electronics)
- **community building & industry involvement**
  - demonstrated added value to industrial projects
  - low entry barrier for new developers and users
  - easy participation of SME / academic groups

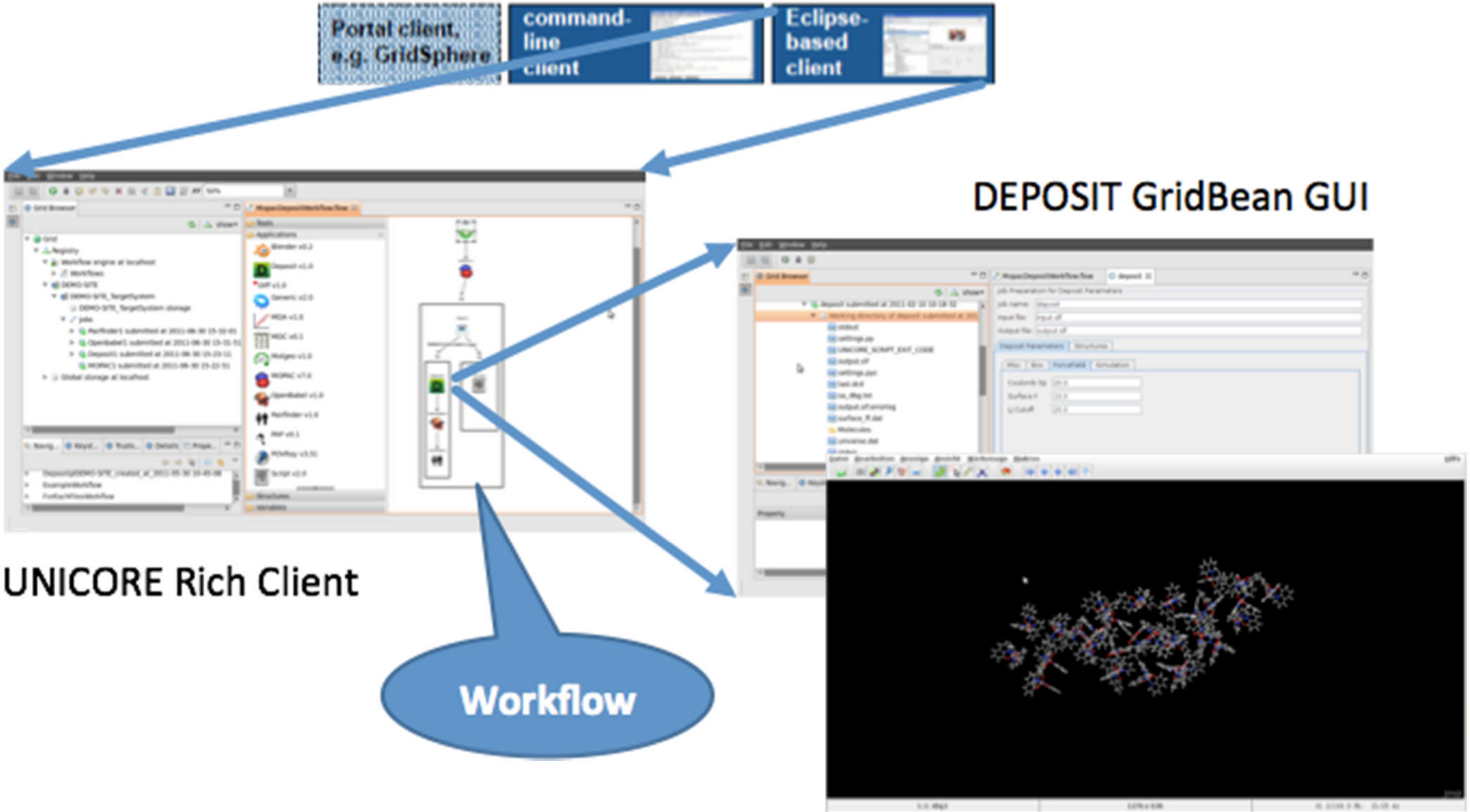
Partners

Participant	Acronym	Country
Karlsruhe Institute of Technology	KIT	Germany
Commissariat à l'énergie atomique	CEA	France
CINECA Bologna	CIN	Italy
CSC - IT Center for Science	CSC	Finland
Korea Institute of Science and Technology	KIST	Korea
Nokia Research Center	NOKIA	Finland
Sony	SONY	Germany
Science and Technology Facilities Council	STFC	UK
University of Mons	Umons	Belgium
University of Patras	UPA	Greece



www.multiscale-modelling.eu

MMM@HPC : From codes to workflows



Available Gridbeans

GridBean + Wrapper	Bundle distributed	IDB configured	Application installed and tested
MOPAC	30/06/2012	15/06/2012	31/05/2012
TURBOMOLE	30/06/2012	15/06/2012	31/05/2012
BigDFT	30/06/2012	15/06/2012	31/05/2012
DEPOSIT	30/06/2012	15/06/2012	31/05/2012
Elmer	30/06/2012	15/06/2012	31/05/2012
DL_POLY	30/06/2012	15/06/2012	31/05/2012
ToFeT (KMC)	30/06/2012	15/06/2012	31/05/2012
End-bridging MC	30/06/2012	15/06/2012	31/05/2012
Transporter	30/06/2012	15/06/2012	31/05/2012
ADF	30/06/2012	15/06/2012	31/05/2012
PairFinder	30/06/2012	15/07/2012	30/06/2012
OpenBabel	30/06/2012	15/07/2012	30/06/2012
MEMPhys	30/06/2012	15/07/2012	30/06/2012

MMM@HPC Concept

MMM@HPC

Reusability
- GridBeans
- UNICORE Workflows

Data complexity
- Chemical Mark-up Language (CML)
- OpenMolGRID

Solution for licensing issues
- UNICORE: UVOS/SAML/VOMS
- Open Source Licenses

Security & Reliability
- UNICORE
- Grid Security Infrastructure (GSI)

Capacity & Capability
- High Performance Computing (PRACE)
- Distributed resources (D-Grid, EGI)

YES!

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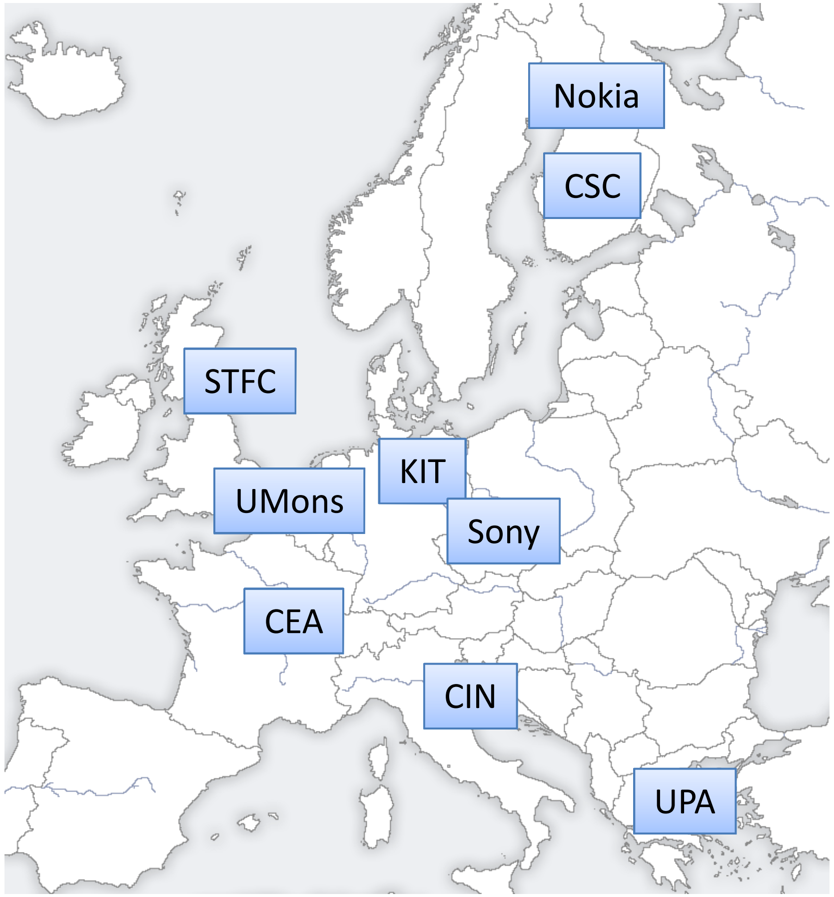
Commissariat à l'énergie atomique	CEA	France
CINECA Bologna	CIN	Italy
CSC - IT Center for Science	CSC	Finland
Korea Institute of Science and Technology	KIST	Korea
Sony	SONY	Germany
Science and Technology Facilities Council	STFC	UK
University of Mons	Umons	Belgium
University of Patras	UPA	Greece



www.multiscale-modelling.eu

MMM@HPC HowTo

- Install the Unicore Rich Client (~ Program Development Tool)
- Get some Gridbeans (Gridbean Repository)
- Get some Computer-Resources
  - Requires Unicore (~ job management system)
  - HPC-Prace Centers: CINECA/CSC
  - Your own cluster: Unicore Live CD
- Build a workflow ….. Push the green button … get a paper
- ….. Modify workflow a bit … Push the green button again … get another paper (…. with another student)
- …… use your friends workflow … get another paper
- Afterwards:
  - Publish the workflow with your paper
  - Deposit new gridbeans in the repository
- www.multiscale-modelling.eu

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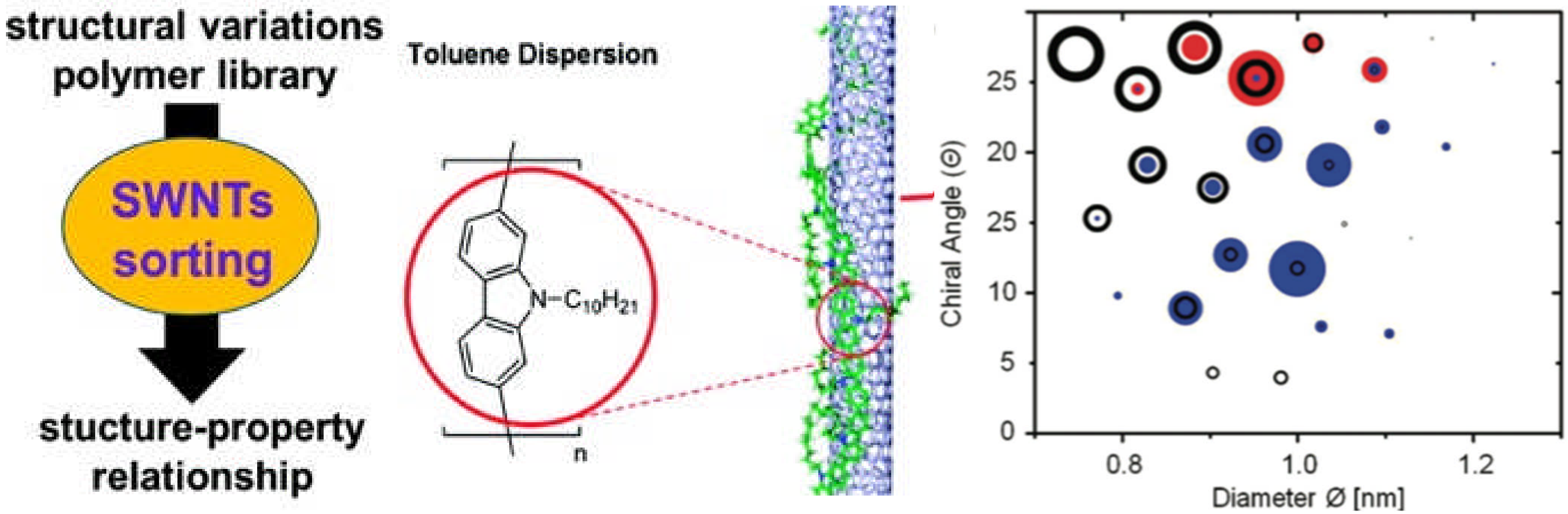
Chirally Selective Solvation of CNT

Use the polymers to selectively disperse CNTs with different radius & chirality

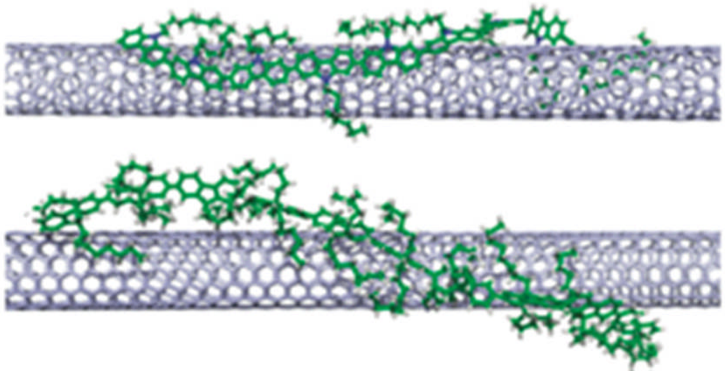


F. Lemasson, T. Strunk, Gerstel, F. Hennrich, S. Lebedkin, Barner-Kowollik,
W. Wenzel, M. Kappes, M. Mayor, JACS, 2011

Modelling Polymer Wrapping of CNT

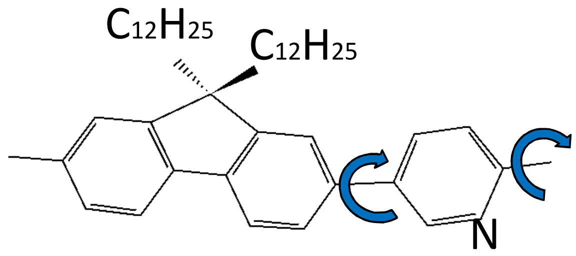
Wrapping polymers with MC simulations:

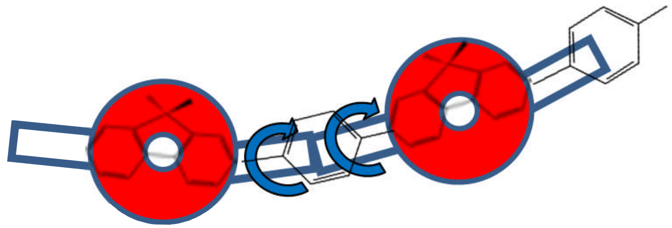
- Scale QM: Polymer Properties
- Scale MM: Energy Relaxation



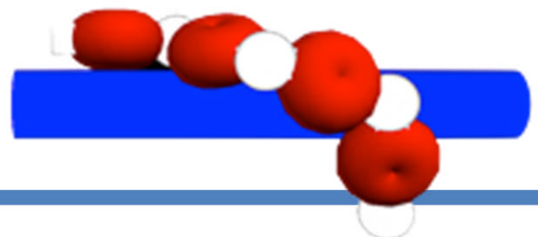
F. Lemasson, T. Strunk, Gerstel, F. Hennrich, S. Lebedkin, Barner-Kowollik, W. Wenzel, M. Kappes, M. Mayor, JACS, 2011

- Coarse grained model





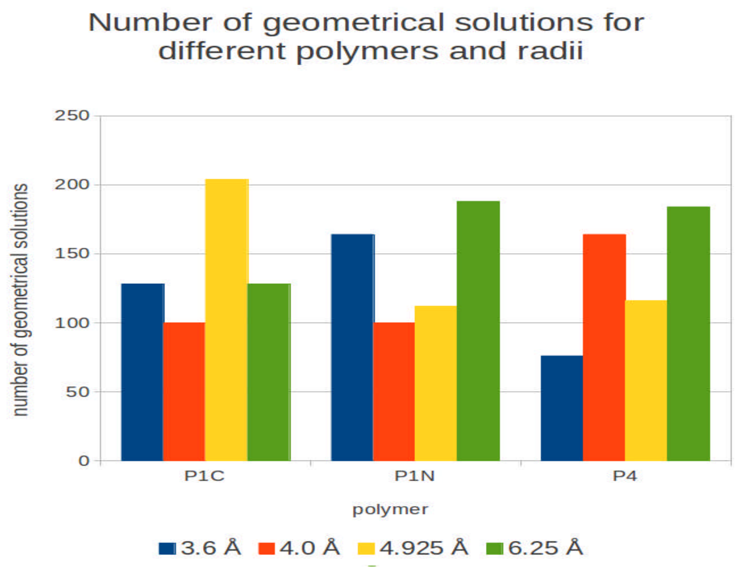
- Recursive analytical construction of solutions

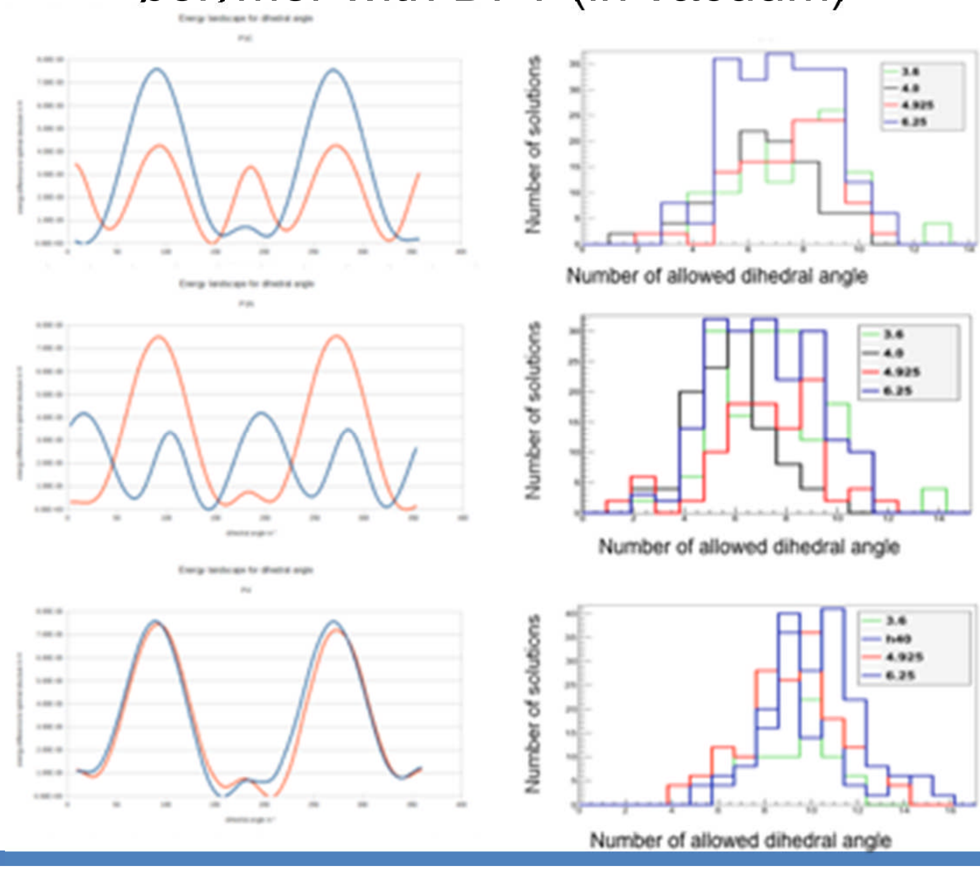


Coarse grained modelling

Number of structures from geometrical model vary with parameter selection

Compare the values of dihedrals to the values obtained for the same polymer with DFT (in vacuum)





P1C

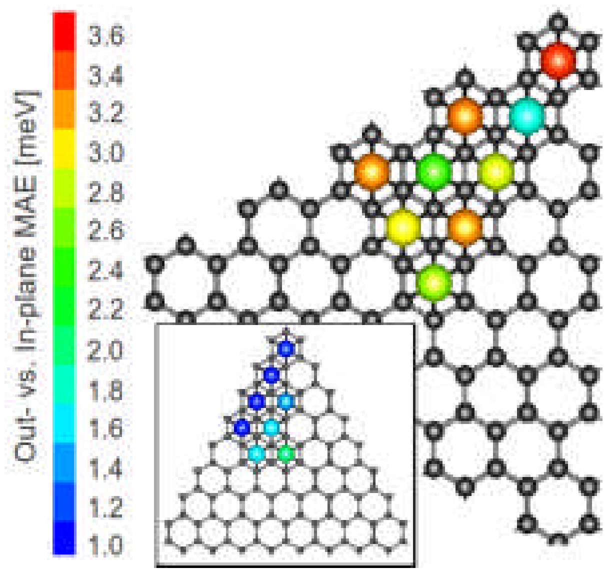
P1N

P4

Further Applications

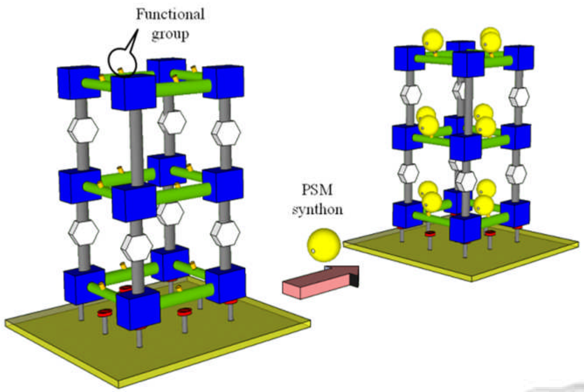
- Magnetic adatoms on graphene flakes

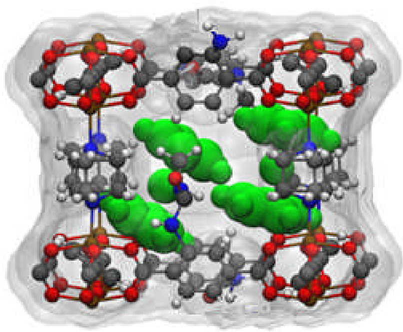
→ I. Beljakov



- Morphology of metal organic frameworks

→ (T. Neumann/AG Wöll)





Summary

- Materials design up to the device level spans many different scales in a heterogenous software landscape
- Multiscale Modelling Toolkits should be
  - Open
  - Adapdable
  - Extendable
  - HPC Ready
- MMM@HPC delivers a Unicore/Gridbean based environment for multiscale simulations
- Gridbeans exist for many popular materials modelling programs

Thanks for your attention

On the road to simulations for predictive in-silico materials design ……..

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  - Magnetic Storage using Graphene Flakes (Poster: I. Beljakov)
  - Electronic Transport through amorphous organic films (Poster: D. Danilov, Talk: V. Meded)