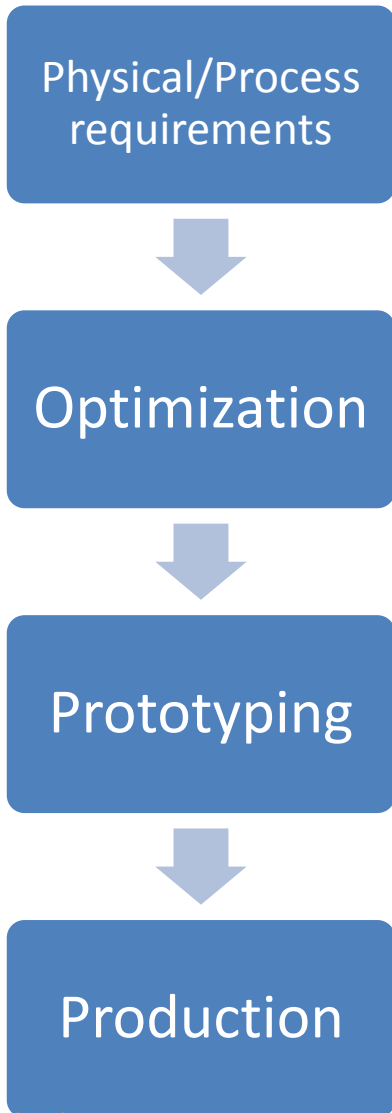


Industrial Applications of Multi-Scale Modeling on Organic Materials

A paradigm shift for the invention and optimization of organic materials



Materials Development Challenges



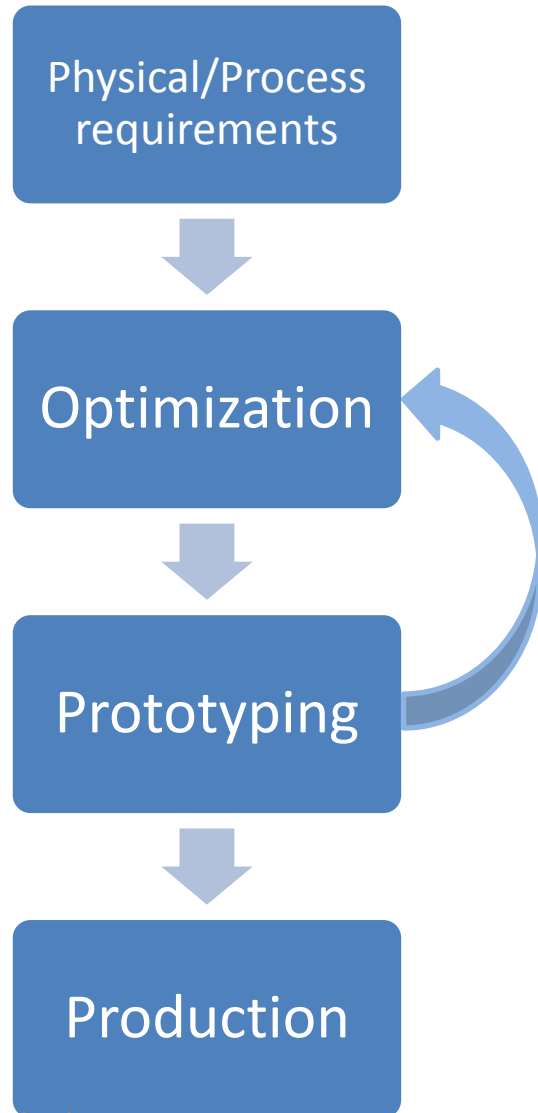
- spectral properties
- morphology
- crystallisation tendency
- solubility
- evaporation temperature

- invention of new materials
- modifications of known structures
- modulation of HOMO / LUMO, mixing ratios

- synthesis
- purification
- prototyping
- testing
- device characteristics

- mass production of speciality chemicals
- R2R process

Materials Development Challenges



The Time Limiting Factor:

R&D success rate

1. Synthesis capacity
2. R&D efficiency



- spectral properties
- morphology
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- invention of new materials
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Automotive Development

Development Time: 18 Months



Success Factors for Industrial Design:



> Modularization

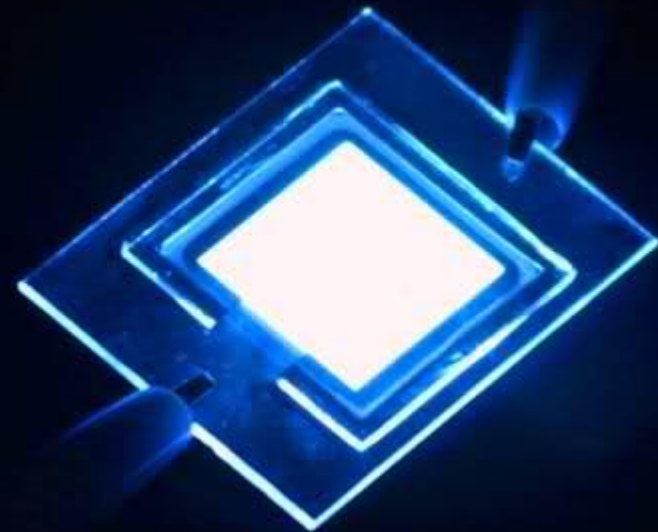


> Automation



> Virtualization





Introducing the Missing Link

Morphology simulation at atomic precision

DFT based charge transfer and electronic properties

- > Targeted optimization of known organic materials and
- > Virtual screening of new charge transfer materials
- > Electronic aging and effects at interfaces
- > Electronic properties of molecules in the matrix

Virtual development of new organic materials

MMM@HPC Success Story

- > MMM@HPC solutions integrated by Nanomatch allow
 - overcoming the time limiting factor in current material development best practices
- > Technology:
 - providing an integrated virtual model of organic electronic materials, material mixtures and material stacks
- > Usability:
 - providing a user friendly, industrial quality material discovery environment for new organic materials
 - Nanomatch is sustaining the MMM@HPC know-how following up the project runtime

Accessing the Technology

Simulation R&D Projects



Standardized Workflows



Technology Platform



Accessing the Technology



Simulation R&D Projects



Standardized Workflows



Technology Platform



Simulation R&D Projects



Coordination of R&D projects including

- > EU partners within the MMM@HPC network
- > Sustain the network of excellence in win-win situation

Components:

- > Unified contract research
- > Custom tailored workflows

Accessing the Technology



Simulation R&D Projects



Standardized Workflows



Technology Platform



Standardized Workflows

Standardized procedures for material screening



> Web-interface for

- Sketch or upload of molecular material coordinates
- Definition of input parameters

> Download results

> *Examples:*

- HOMO/LUMO Energies (Host/Guest/Matrix)
- Disorder parameters
- Morphologies
- Mobilities

Accessing the Technology



Simulation R&D Projects



Standardized Workflows



Technology Platform



Accessing the Technology Platform

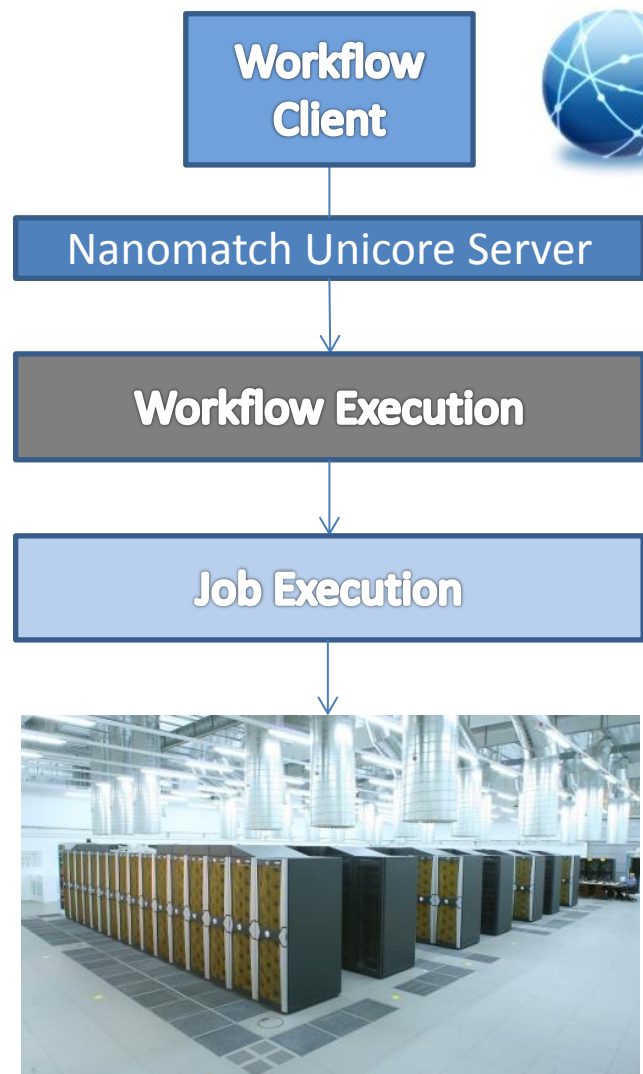
The Nanomatch technology platform is based on the scalable gateway architecture UNICORE.

The infrastructure is:

1. Open
2. Secure
3. Diverse
4. Modular
5. Adaptable
6. Sustainable

Clients can rely on a versatile workflow client with an intuitive user interface to be productively extended and sustained in all day R&D usage.

9/25/2013



Accessing the Technology Platform

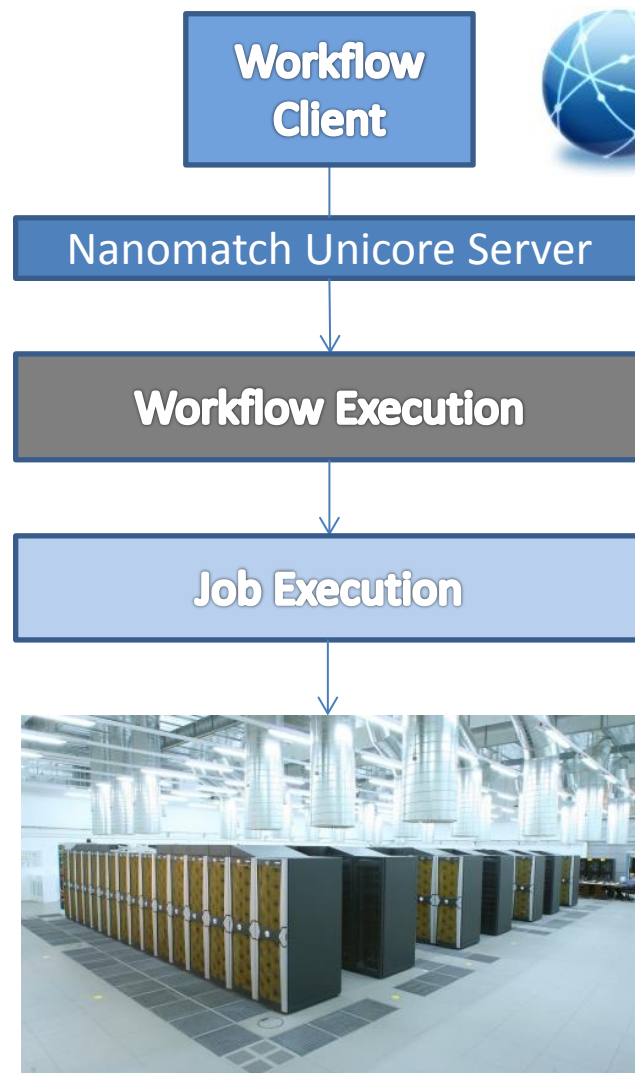
Nanomatch provides an all-in-one high performance computation technology platform even for demanding molecular calculations

Nanomatch provides:

1. Workflow client setup
2. Software licensing
3. Cloud services
4. Maintenance
5. Software GridBean incapsulation
6. Availability

Unique industry scale materials discovery environment.

9/25/2013



Bridging the Gap

Bridging the technological gap:

- > from nanoscaled morphology to the electronic structure

Bridging the informational gap:

- > R&D project planning, paper work and book-keeping can be outsourced
- > integration of academic contributions into unified, custom tailored R&D projects
- > sophisticated multi-scale material simulations can be maintained by non-specialists as workflows

The Assets Provided by Nanomatch

Comprehensive virtual model of the performance attributes of organic material systems

- > transferring industrial design success principles
- > sustaining the know-how of MMM@HPC

Synchronization of co-development cycles in material research

- > overcoming the time-limiting trial&error iterations
- > faster time to market

Virtual screening for new organic materials

- > integrating the organic material discovery environment
- > patent strategy



Nanomatch is a spin-off project supported by
KIT and the Helmholtz-Association.

Our expertise is multi scale materials modeling
targeting amorphous organic thin films.

simon.widmaier@nanomatch.com



GGC
Consulting