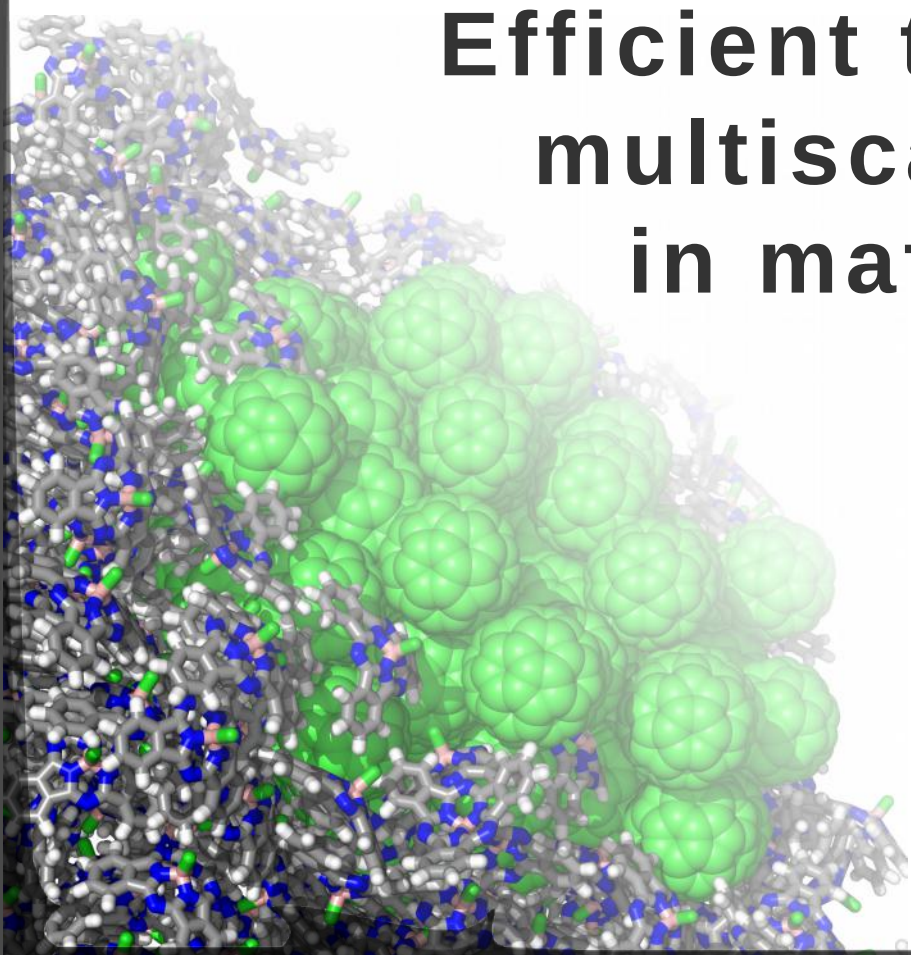


EMMC workshop, 18.09.2017, Warsaw

Efficient translation of multiscale modeling in material research



NANOMATCH GMBH

Eggenstein-Leopoldshafen

www.nanomatch.com

info@nanomatch.com

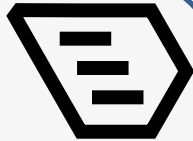
+49 721 608 26884



Virtual Materials Design by Nanomatch

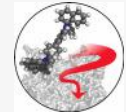


SimStack

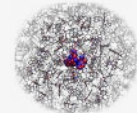


- Generic workflow environment
- efficient incorporation of third-party modules
- Fast implementation of complex workflows

Organic Electronics



- Predictive Software
- State of the art Science
- Consulting



The OLED-Workflow: EXTMOS MODA



See talk by
Thierry Deutsch

1. Single molecule parametrization (QM)

- Geometry optimization
- Customized force-fields

2. Generation of atomistic morphologies

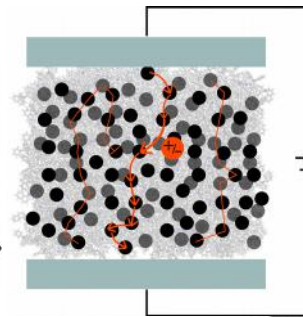
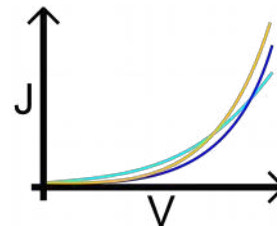
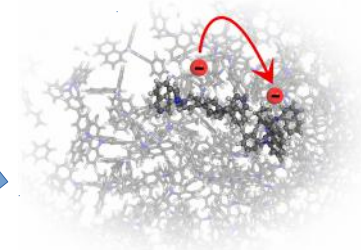
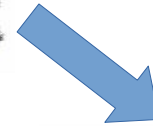
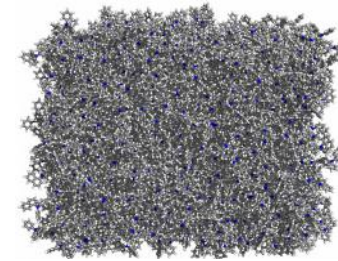
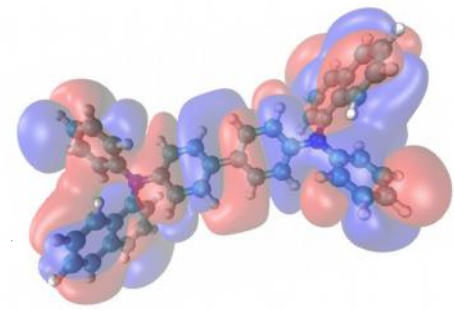
- Molecules parametrized on quantum mechanical level
- Simulation of physical vapor deposition

3. Calculation of charge hopping rates

- Full quantum mechanical electronic structure analysis
- Electronic couplings, reorganization and orbital energies

4. Charge transport simulations

- Time resolved charge carrier trajectories
- Percolation path identification



The OLED-Workflow: EXTMOS MODA



1. Single molecule parametrization (QM)

- Geometry optimization
- Customized force-fields

2. Generation of atomistic morphologies

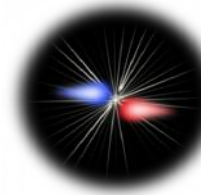
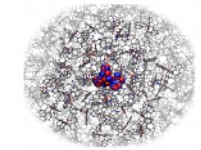
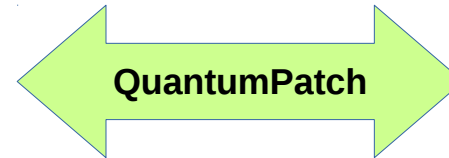
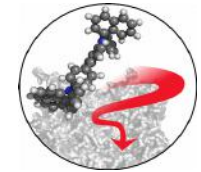
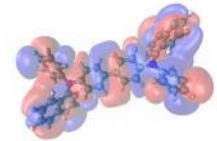
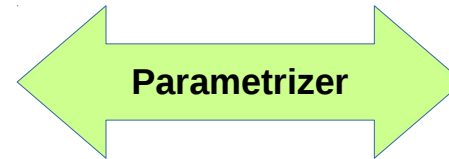
- Molecules parametrized on quantum mechanical level
- Simulation of physical vapor deposition

3. Calculation of charge hopping rates

- Full quantum mechanical electronic structure analysis
- Electronic couplings, reorganization and orbital energies

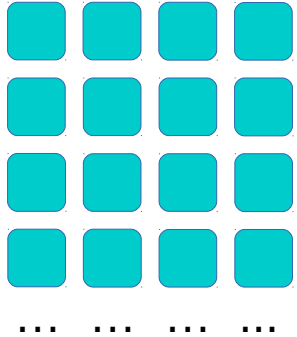
4. Charge transport simulations

- Time resolved charge carrier trajectories
- Percolation path identification

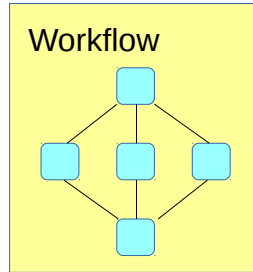


Translation of Materials CAD to Industry

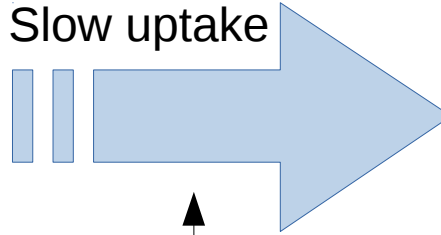
Scientific Modules
EU ROMM



MODA



Slow uptake



End User



???



Three years “lost in translation”

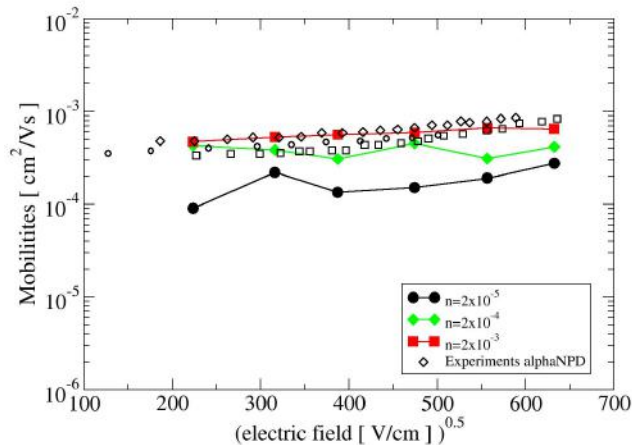
- Accuracy & reliability of methods
 - General skepticism towards modeling methods
- Highly sensitive IP
 - Companies do not disclose promising compounds, systems or even pressing problems/questions
- Costs
 - Up-front investments and running expenses limit ROI



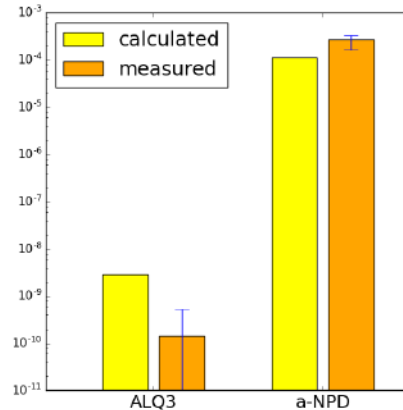
Translation barrier #1: Accuracy & reliability

Solution: meet initial scepticism in computational approaches with convincing use cases:

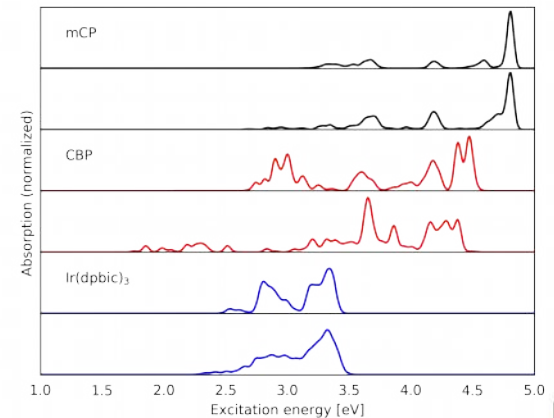
Field dependence of bulk mobility



Charge carrier mobility of pristine layers



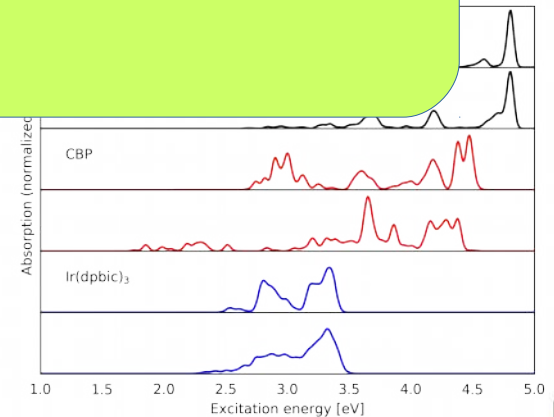
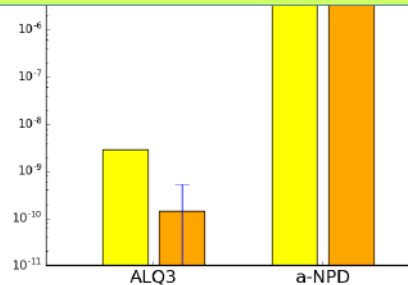
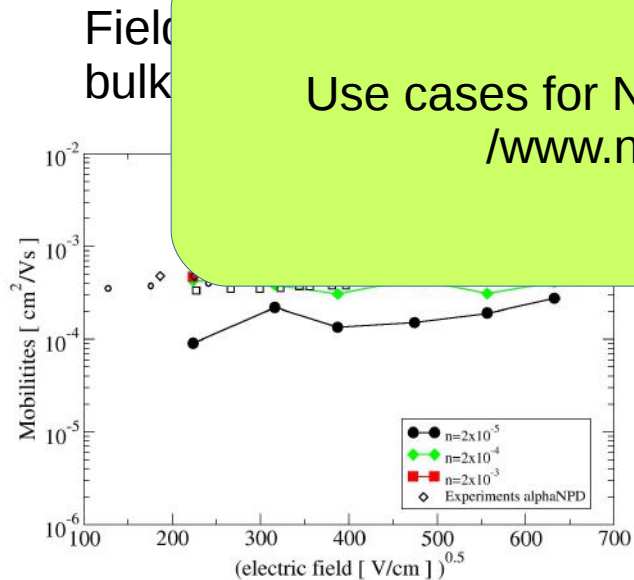
Excitation spectra of embedded molecules



Translation barrier #1: Accuracy & reliability

Solution: meet initial scepticism in computational approaches with convincing use cases:

Use cases for Nanomatch modules available on our homepage:
[/www.nanomatch.com/index.php/en/use-cases](http://www.nanomatch.com/index.php/en/use-cases)



Translation barrier #2: IP

Initial strategy: consultation

- Expertise @ Nanomatch
- Computation @ Nanomatch
- Results delivered to customer in form of reports

No investment in specialized personnel

Minimal training for customer

No investment in hardware

Case 1 (2015-2016):

- German SME
- Prepared specialized use cases
- In contact for 3 years
- Problem: We do not know what exactly they need!

Case 2 (2016):



- Global player
- Established collaboration
- Custom tailored solutions verified for „similar“ systems
- Problem: protected systems require modified approach that is hard to guess



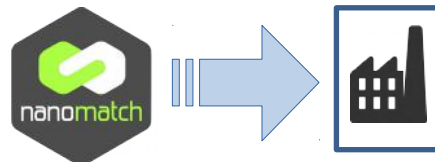
Translation barrier #3: Costs



Incorporating modeling into R&D requires:

- Hardware (100k€ for reasonable HPC stack) 
- Personnel:
 - Experts for multiple methods (150k/a) 
 - Setup and maintenance of HPC resources (120k/a)
- Software licenses
- Time: Expenses only justified if modeling speeds up in R&D significantly

Possible Solution: Consultation?



Translation barrier #3: Costs



Incorporating modeling into R&D requires:

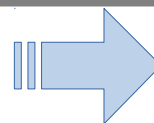
- Hardware
- Personnel
 - Experience
 - Setup
- Software
- Time: Expensive

Case 1 (2017):

- European SME
- Interested in methods and software
- License fees no issue
- Problem:
 - Runtime of 1 OLED simulation: 1 day on 1000 cores
 - Estimated runtime at client HPC: 5 days
 - „We are better off trusting a chemists intuition than waiting 5 days for results“

Possible Solutions

significantly



Successful translation of modeling methods

What we learned:

- 1) Application by the industrial researcher is essential due to IP
- 2) Modeling needs to generate obvious added value within the company
- 3) Faster or more results than by experimental trial and error

Modeling software needs to ...

... be easy-to-use

... allow
high scalability and
reproducibility

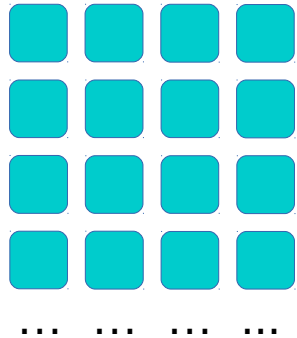
... provide a high
level of predictivity
and reliability

... be supported by webinars and hands-on tutorials to reduce initial barriers

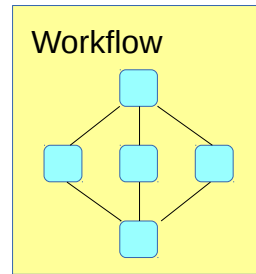


Translation of Materials CAD to Industry

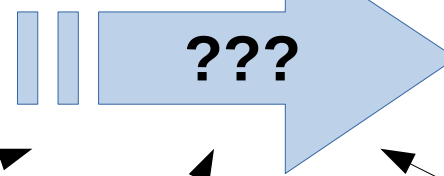
Scientific Modules
EU ROMM



MODA



Slow uptake



End User



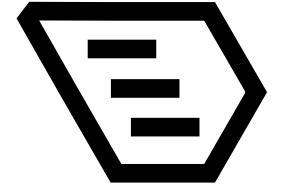
No market ready tool:
Custom tailored solution
for each specific problem
needed!

Low scalability of case-to-
case patchwork solutions
annihilate advantage over
experimental trial & error

Scalable computational
resources are hard to
access / configure

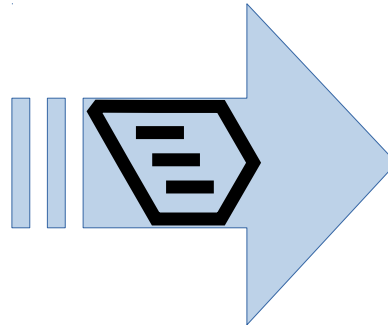
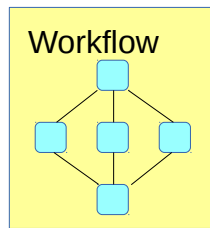
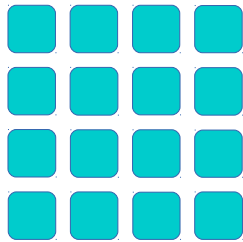


Translation by SimStack



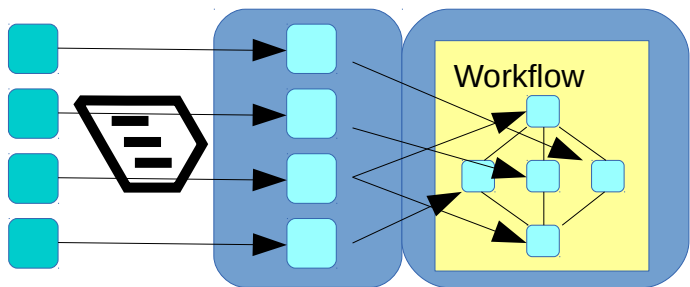
... a generic workflow platform conquering complexity

- open to arbitrary software modules
- rapid prototyping: 30min to include new modules, 1 h to construct functional workflows
- maximal reusability and scalability

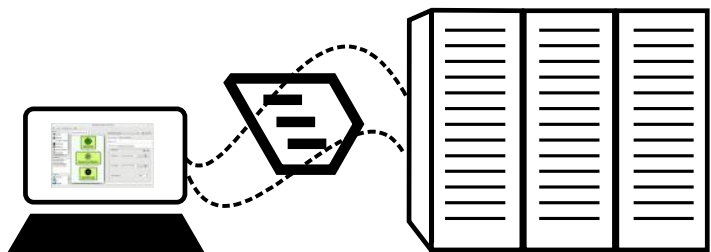


SimStack workflow platform

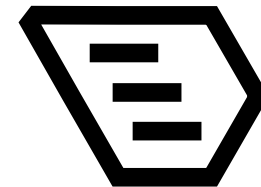
Efficient translation into scalable, re-usable workflows



One-click execution of workflows on HPC facilities

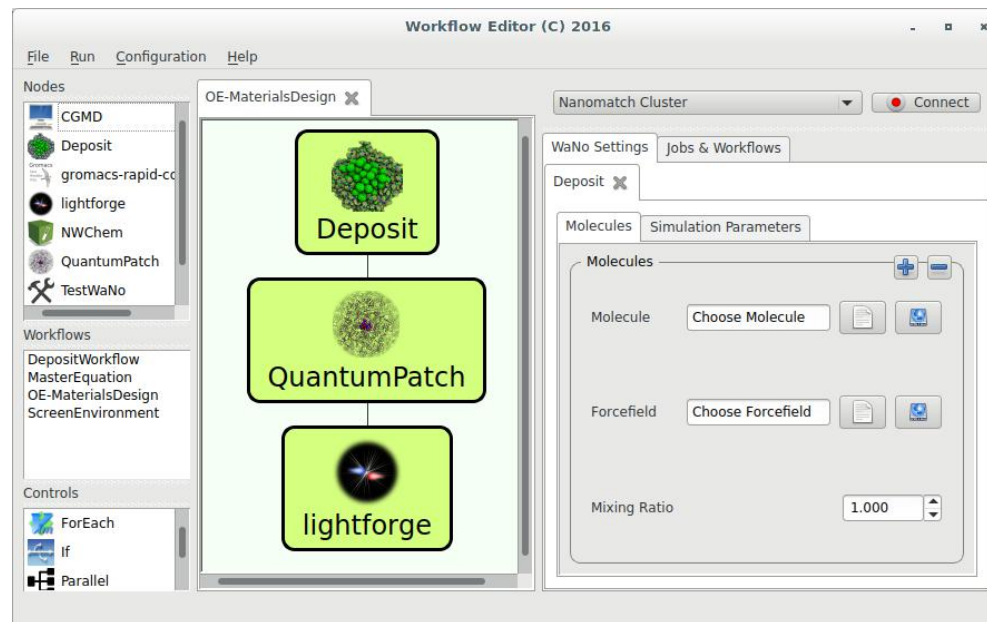


SimStack workflow platform

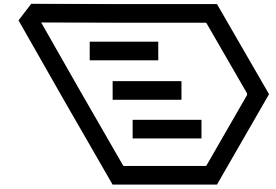


Key Features

- Quick incorporation of modules
- Drag&Drop workflow engineering
- Automated HPC handling
- Automated module interfacing
 - Rapid prototyping of complex adaptive workflows



SimStack workflow platform



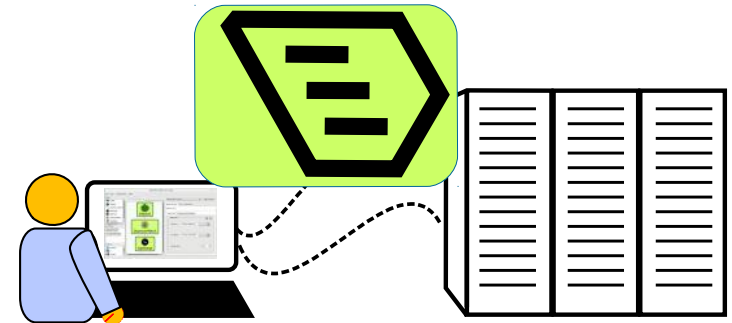
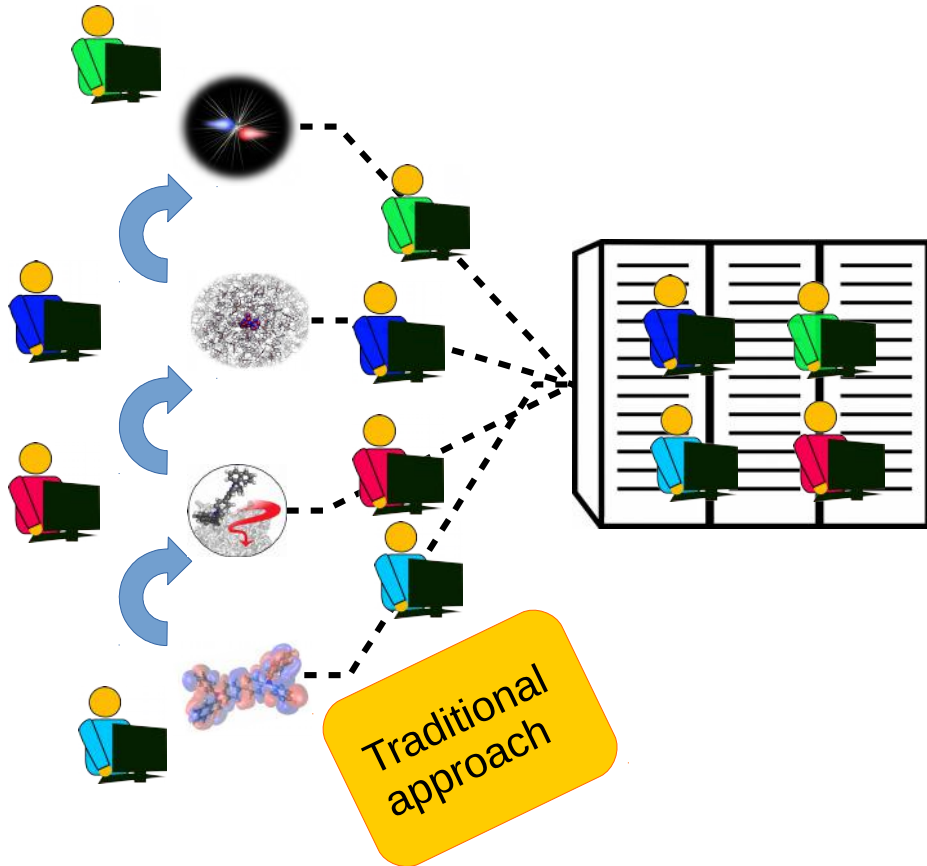
Key Benefits for the end user

- Competitive edge components
- Hidden complexity of HPC handling
- Easy-to-use scientific modules
- Highly scalable usage of complex simulations
- Light end-user installation due to special client-server-setup



Conquering Complexity

Tutorial and
demo:
15:15h

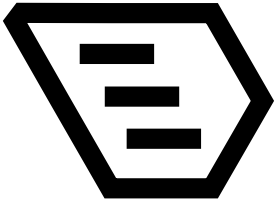
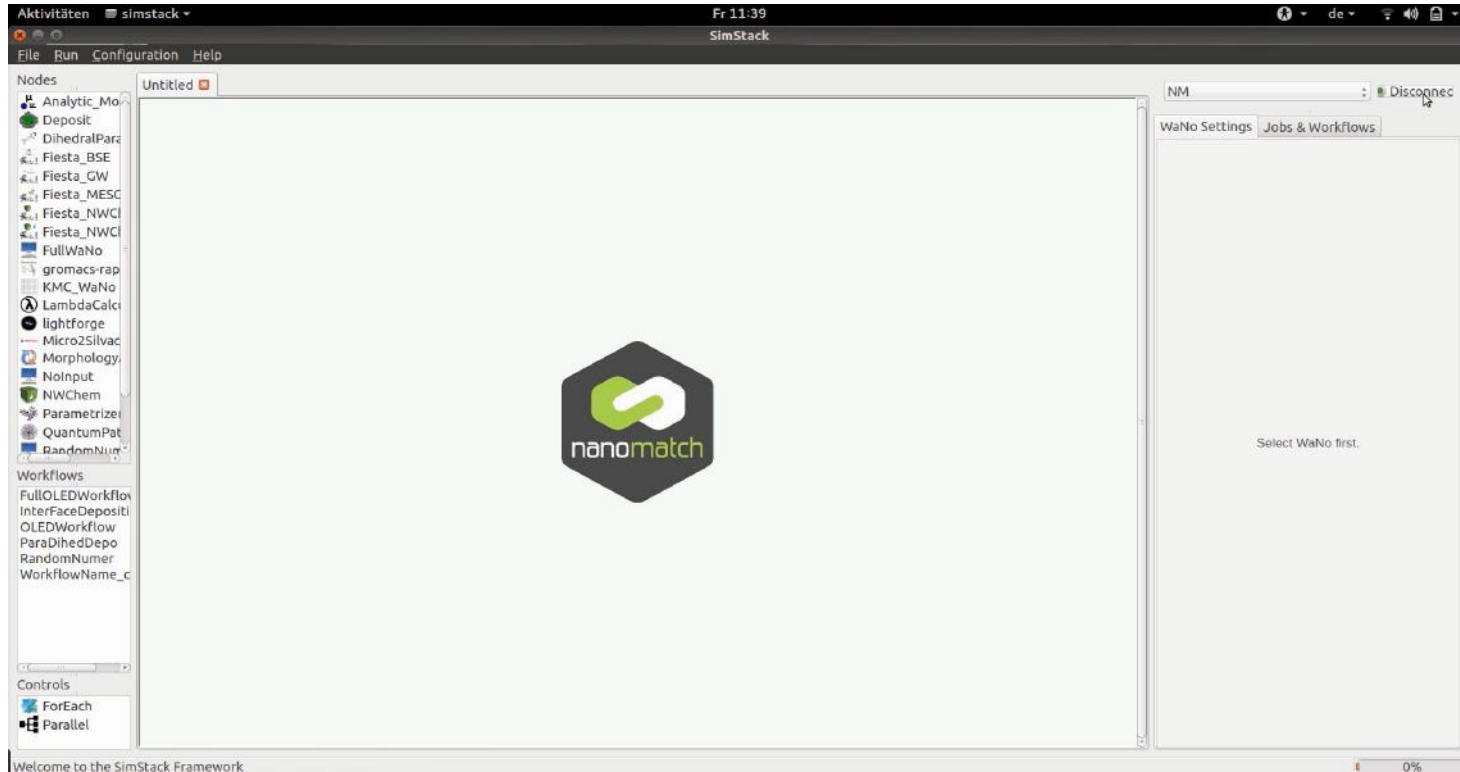


- Scalability
- Throughput
- Reproducibility
- Flexibility



The OLED-Workflow with SimStack

Tutorial and
demo:
15:15h



<https://youtu.be/VBxEYiZv7f8>



Transfer of Materials CAD to Industry

