

A background image showing a complex molecular simulation. On the left, there is a dense cluster of atoms represented by small spheres in grey, blue, and red. On the right, there is a large, green, multi-lobed structure that resembles a protein or a complex molecule, rendered in a semi-transparent style.

Challenges in the Translation of materials modeling techniques to industry



14.06.2016, Glasgow

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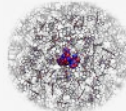
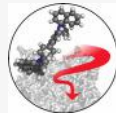


Virtual Materials Design by Nanomatch



Organic Electronics

- Predictive Software
- State of the art Science
- Consulting



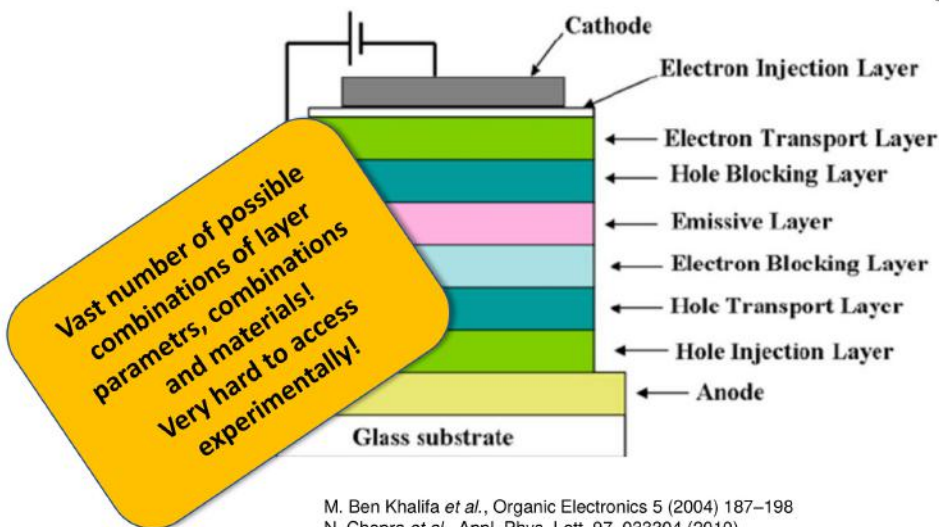
SimStack

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

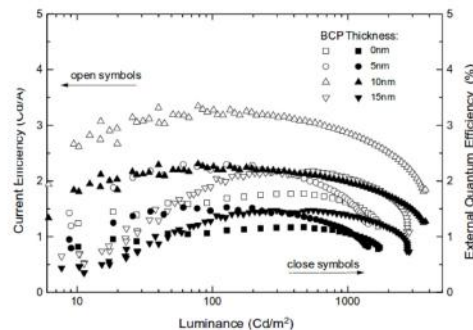
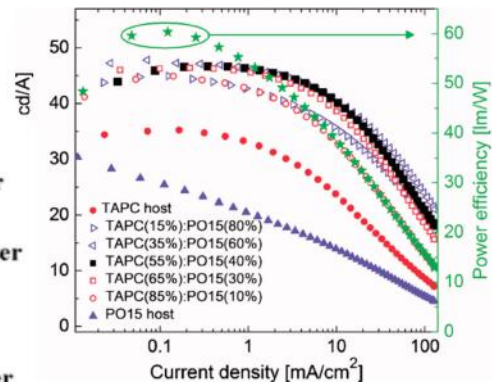


Challenges in Organic Electronics

OLED challenges



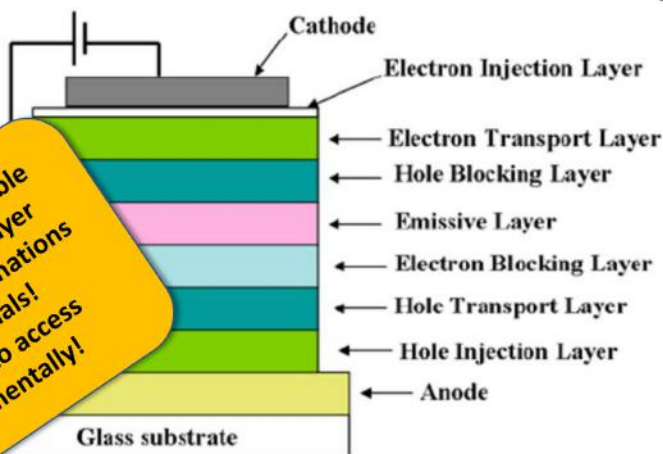
M. Ben Khalifa *et al.*, Organic Electronics 5 (2004) 187–198
N. Chopra *et al.*, Appl. Phys. Lett. 97, 033304 (2010)
R. Srivastava *et al.*, Organic Light Emitting Diode, ISBN 978-953-307-140-4



Challenges in Organic Electronics

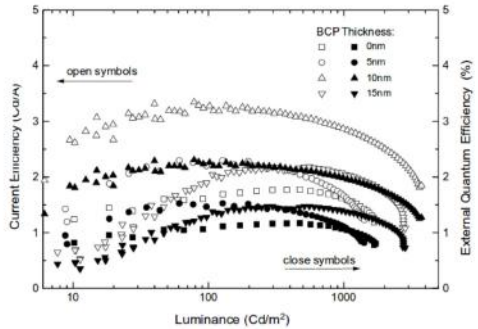
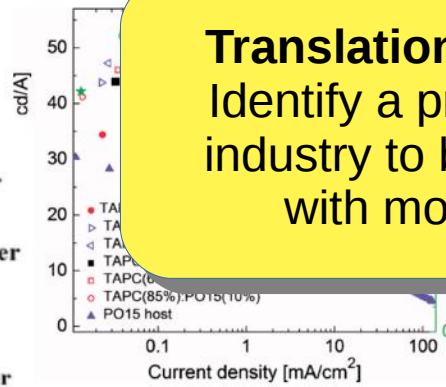
OLED challenges

Vast number of possible combinations of layer parameters, materials and materials!
Very hard to access experimentally!



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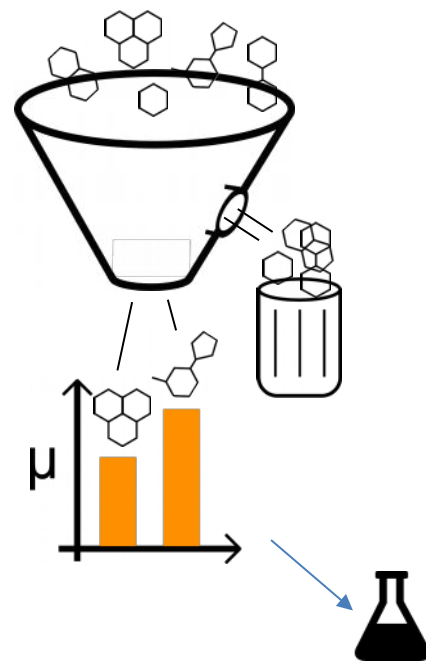
Translation step #0:
Identify a problem in industry to be solved with modeling



Predictive device simulations → CAD in OE



- Automated bottom up multiscale modeling on HPC architectures
- **Parameter free** simulations on the device level
- Efficient **identification of bottlenecks** in device performance
- **Virtual optimization** of compounds for various applications



Translation Case: facilitating CAD in OE



Benefits for users:

- Stack simulations as virtual microscope
- Efficient screening of system parameters
- estimated ROI: ~ 7 - 10

Clients:

- Manufacturers of OLED devices
- Developers of chemicals used in OLED devices

Translating modeling methods...

- As a service provider
- As a software provider



Translation Challenge: Bringing parameter-free OLED modeling methods to industry

High level of complexity



KIT
Karlsruher Institut für Technologie

Methods developed and implemented in various Diploma/Master and PhD projects since 2010

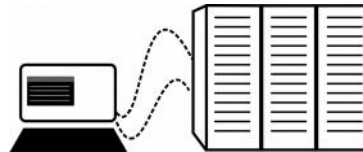
Diverse specialized expertise required

Physical effects on multiple scales



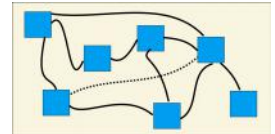
- Quantum Chemistry (DFT)
- Molecular Modeling (Force fields, MD, MC)
- Charge transport simulations (KMC)

HPC expertise



- Accessing HPC resources via command line
- Setup of submission scripts (Linux, shell)
- Running and monitoring jobs on 100+ CPUs

Information transfer between modules

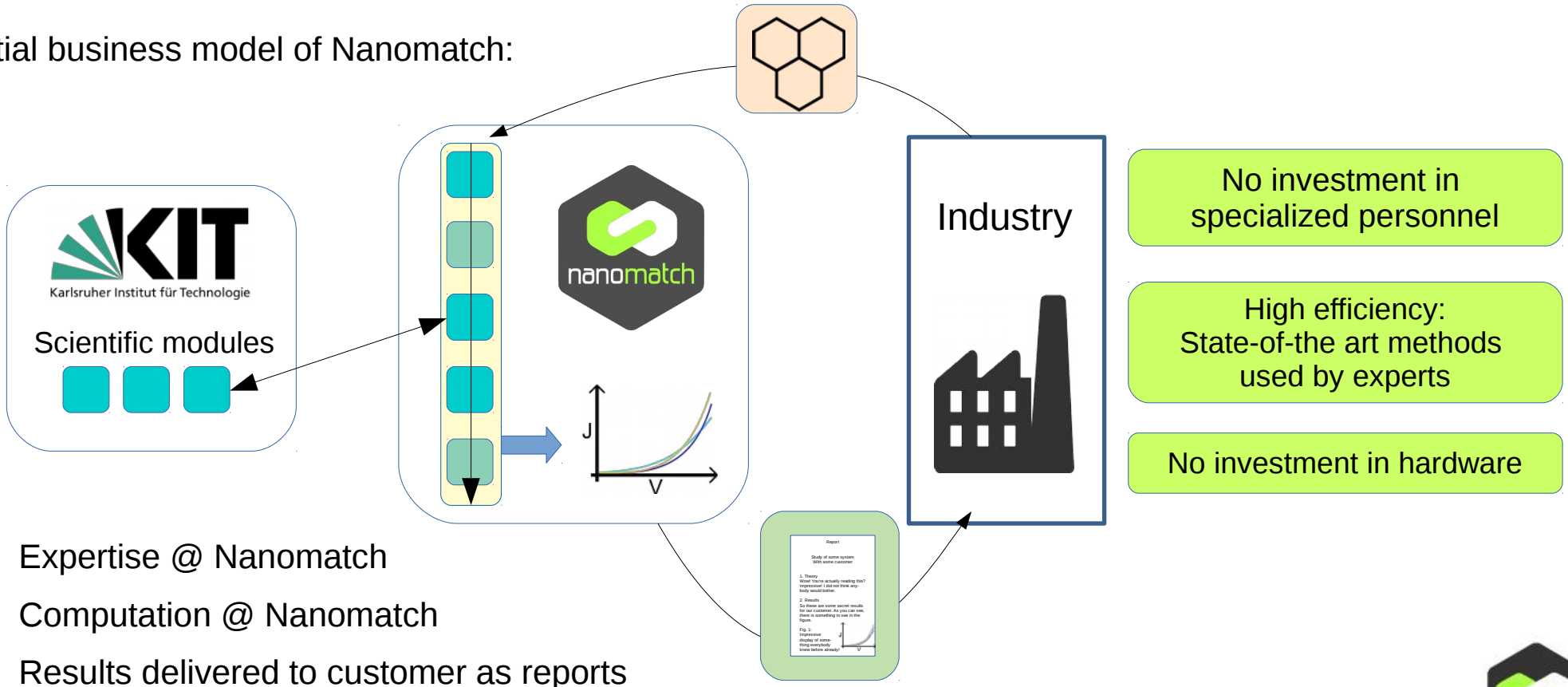


- File conversion scripts
- Modification of folder structures
- Analysis scripts



Evolution of a business model

Initial business model of Nanomatch:



- Expertise @ Nanomatch
- Computation @ Nanomatch
- Results delivered to customer as reports



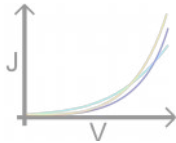
Evolution of a business model

Initial business model (2015-2016):

Case 1 (2015-2016):

- German SME
- Prepared specialized use cases
- In contact for 3 years
- Problem: Specific questions to be addressed by modeling cannot be disclosed to service providers

Scientific modules



Industry



No investment in specialized personnel

High efficiency:
State-of-the art methods used by experts

No investment in hardware

- Expertise @ Nanomatch
- Computation @ Nanomatch
- Results delivered to customer as reports

Report

State of service system with your customer

1. Theory
Small "Hello world" example that demonstrates I did not drink any body modification.

2. Results
On these data some secret results for your customer, who you can see from the following figure in the figure.

Fig. 1
Performance
Graph of some
very beautiful
data showing strategy.



Evolution of a business model

Initial

Case 1 (2015-2016):

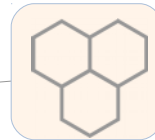
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Scientific modules

Case 2 (2016):

- Global player
- Established collaboration
- Custom tailored solutions verified for systems from the public domain
- Problem: Information on protected systems cannot be provided

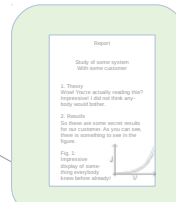
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No investment in specialized personnel

High efficiency:
State-of-the art methods
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Evolution of a business model

Initial

Case 1 (2015-2016):

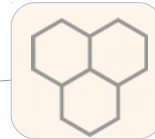
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Scientific modules

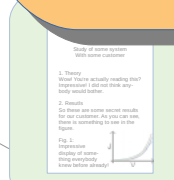
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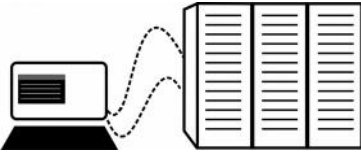






Sensitive IP demands application of modeling software by industrial end-user



Running the software is expensive

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 


Case 3 (2017):

- European SME, Interested in methods and software, License fees OK
- Problem:
 - Runtime of 1 full 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“



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 ...

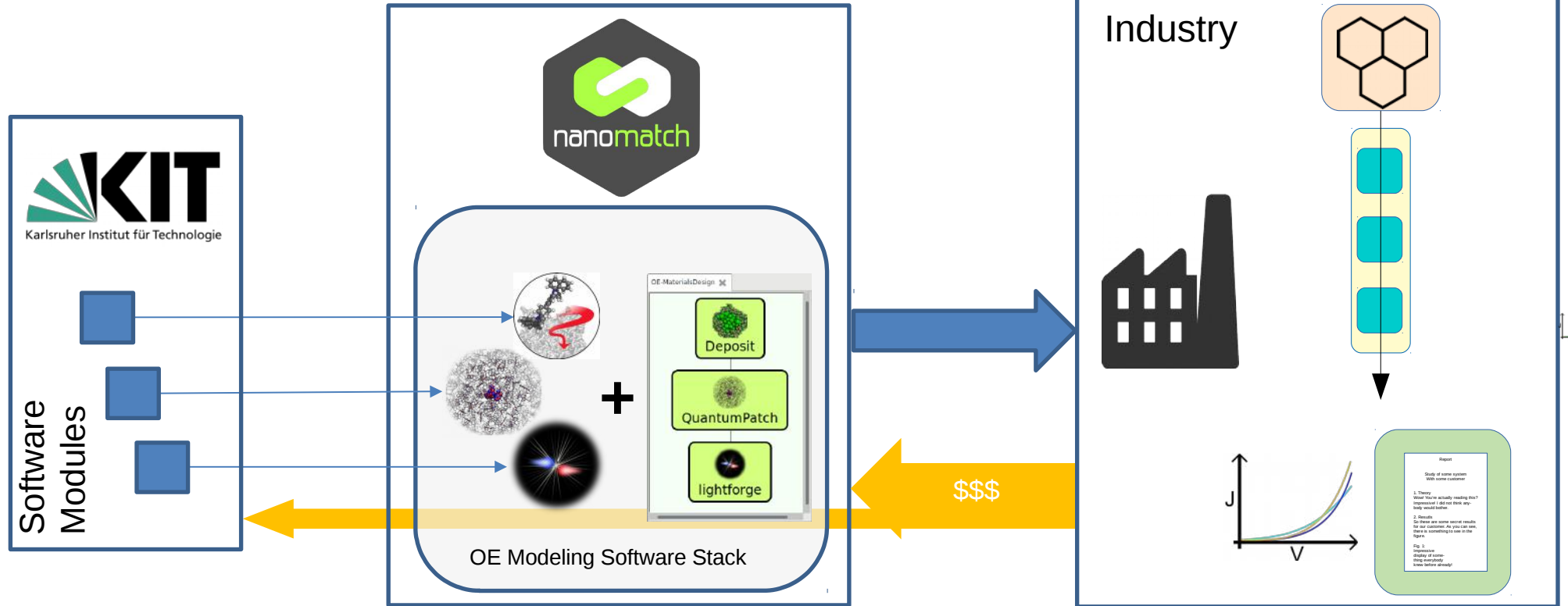
... be easy-to-use

... allow high
scalability and
reproducibility

... be adaptable on a
case-to-case basis



New business model: marketing easy-to-use software solutions



New business model: marketing easy-to-use software solutions

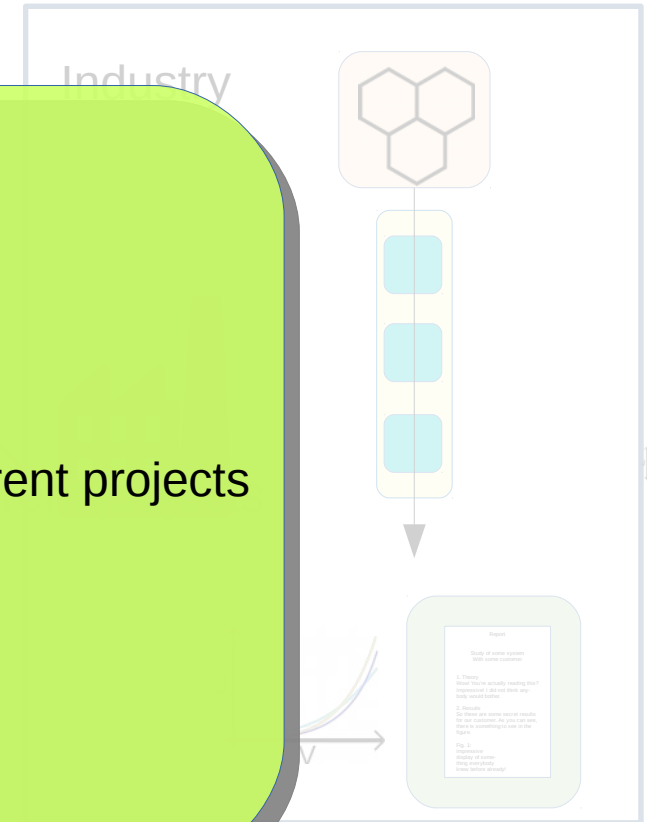
Benefits of the new business model:

For the end-user:

- Sensitive IP stays in-house
- Clients can flexibly apply modeling in different projects
→ **Increased impact of modeling**

For Nanomatch:

- Scalable product

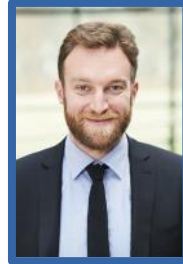
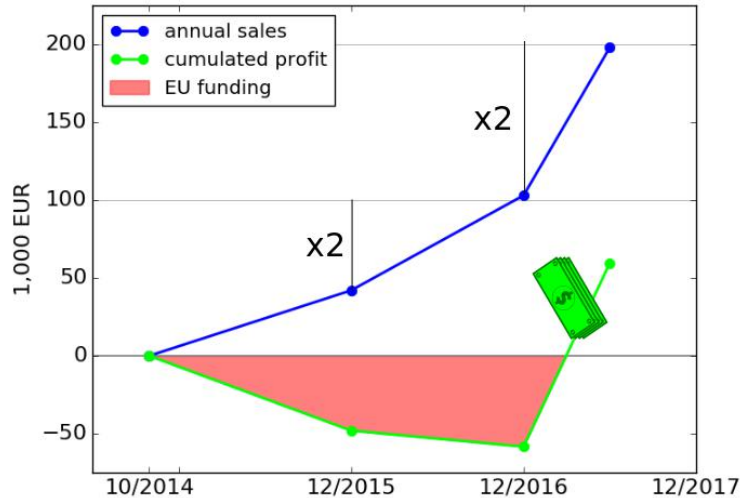


Translation steps

- | | |
|---|-------------|
| 1) Development of reliable modeling methods | 2008 – now |
| <ul style="list-style-type: none">- Validation against experiments- Publish use cases and scientific papers | |
| 2) Advanced software development / engineering: | 2014 - 2017 |
| <ul style="list-style-type: none">- Turn academic code into marketable tool- Installers and license servers- Runtime stability & error handling | |
| 3) Reduce complexity for the end-user | 2016 - 2017 |
| 4) Provide documentation and training material: | 2017 - 2018 |
| <ul style="list-style-type: none">- Use cases, functionality specifications- Online tutorials and webinars | |



Four+ years of translating OLED modeling methods



Tobias Neumann
CEO



Timo Strunk
CTO



Franz Symalla
Principal Scientist



Wolfgang Wenzel
*Scientific Consultant
Member of the board*

- Founded in April 2014
- Profitability after 2 ½ years
- From 1 FTE to 5 FTE by 12/2018
- Industry leading customers
- Participation in EU projects

