EMMC Translation Case: Nanomatch GmbH

Introduction

Translator Profile

Nanomatch is a Software Company (SME) located in Germany. We provide predictive & parameter-free simulation tools for virtual materials design and computer based device optimization in organic electronics, implemented in a seamless workflow using electronic, atomistic, and continuum models. Additionally, we developed a generic workflow platform for the efficient translation of complex multiscale simulation approaches with modules from many sources into market ready tools for industry.

Client

The client is a large, globally active enterprise consisting of several subsidiaries, and develops and manufactures organic electronic materials and devices. Our software and services are mainly used in the enterprise's internal basic research unit. We have an ongoing collaboration with the client.

Industrial/Business Case

The vast number of stable chemical organic compounds and the variety of system parameters (number of layers, layer thicknesses, doping concentrations, etc.) makes the identification of perfect material combinations and device parameters via experimental trail & error a time-consuming and costly endeavour. Furthermore, many processes and properties on the electronic scale cannot be observed in experiment and inhibit a targeted approach to device design.

In contrast to other branches such as the automotive or aerospace industry where computer aided design is a major pillar in R&D, development of novel materials and devices in organic electronics (OE), namely organic photovoltaic (OPV) devices or organic light emitting diode (OLED) applications (such as displays), relies strongly on time consuming and costly experimental trial & error approaches. One of the fundamental reasons therefore is the lack of a single model/module that computes properties of complex multilayer devices, solely based on information on the chemical compounds that are used in the devices. This is overcome by combining multiple models on the electronic, molecular and device scale into a seamless, predictive multi-scale workflow. As the computation of properties and processes in organic electronic layers and devices is still subject to academic research, this also includes modules of academic state-of-the-art modules.

To establish modelling in the client's R&D, the client allocated a lower six-digit sum for software and consultation, plus personnel costs (presumably 1-2 FTE). The expected outcome of the translation process was the large-scale in-house application of state-of-the-art models by the client, in order to allow simulations on systems that include proprietary materials (which wouldn't have been possible if simulations were conducted as a service by us). While we maintain an ongoing collaboration with the client to develop custom-tailored solutions including the latest methods, the first translation period was 12 months.

Translation to modelling solution

Established solutions for OE, such as Drift Diffusion or Finite Element solvers, rely on parametrised models, limiting computer aided design in two ways: First, these models need to be calibrated using experimental data and hence impede full virtual design. Second, no information on the electronic

scale that is crucial for a fundamental understanding of the impact of specific microscopic processes and effects on device properties is provided by these models. This understanding, however, is essential for the targeted design of compounds and devices.

We therefore used the multiscale approach, where information on the electronic scale (quantum mechanical computations of molecules) is transferred via the atomistic scale (molecular layers) to the device scale in four simulation steps. This parameter-free approach eliminates the necessity of experiments prior to simulation, as no experimental input/calibration is needed. This approach is illustrated in Fig. 1. As there was no module for step 4 at the beginning of the collaboration, only modules for steps 1-3 were provided to the client. Starting on January 1st 2018, this last step, as well as improved modules for steps 1-3, are provided in the ongoing collaboration.

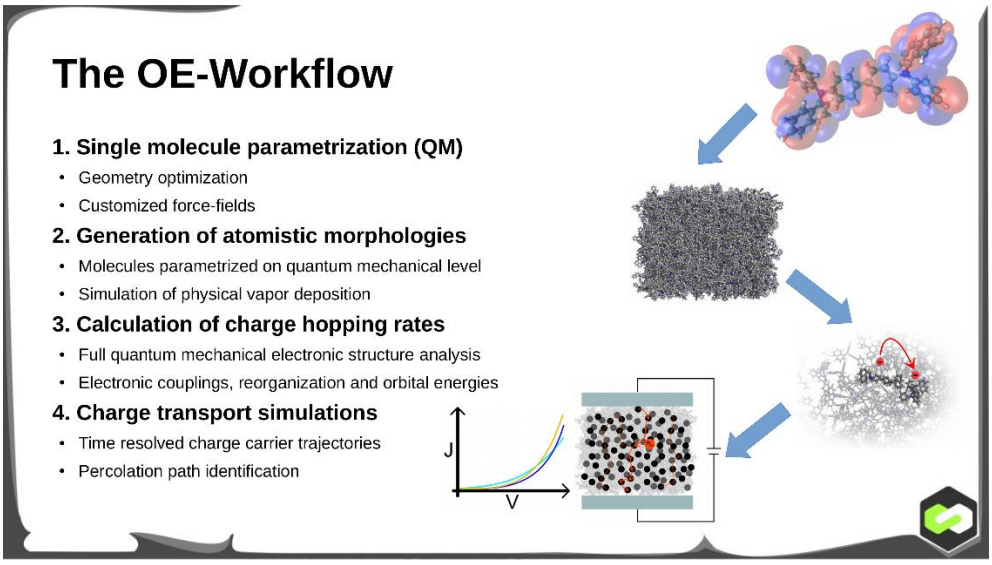

Figure 1: Multiscale workflow for predictive OLED or OPV simulations.

The simulation outcome can be validated at several stages: After step 2, properties of molecular layers, such as density or radial distribution function, can be compared to experimental data. Step 3 provides information on the electronic structure, namely orbital energy levels, that is also accessible via experiment. Finally, charge carrier simulations provide macroscopic device properties such as I-V curves, that can be easily measured in experiment. Possible validation steps and expected levels of accuracy were discussed with the client. However, to protect ongoing research and IP, no information on the performed validation steps or their outcome was disclosed to us by the client.

We recently entered negotiations with the client for the development of specific features to increase model accuracy. For the implementation of the module extensions, the client will invest a sum in the lower six-digit range over the course of 12 months. The decision on models, their exact features and necessary extensions is therefore subject to ongoing research collaborations. We expect this to continue over the next years, as it is essential to maintain a competitive edge over competing approaches by staying at the state-of-the-art level of academic research. New features are then developed by Nanomatch using compounds and systems in the public domain, before providing stable releases to the client for application to proprietary systems.

Client's benefits from the modelling

While the client did not disclose any simulation results to us, we are aware that the simulations were conducted to develop a fundamental understanding of processes and effects in OE layers and devices. This understanding will help to improve device performance, thereby contributing to innovation on a long-term scale and helping to secure and improve the client's position in the market. By incorporating modelling at this early stage in the product design process, the client is able to avoid dead ends and limit the efforts spent on experimental trial&error approaches, saving time and money and, most importantly, allowing shorter time to market. A quantitative estimate for the client's benefits, such as ROI or cost savings, is hard to achieve both due to the limited information and the time scale at which an impact on market share and sales can be observed.

Evaluation of the translation case

As indicated above, there are several bottlenecks in the translation process, that we also encountered with other clients:

- Modelling accuracy and applicability: The applicability of the individual methods implemented in the first version acquired by the client was demonstrated in various scientific publications. However, it is necessary to constantly incorporate state-of-the-art approaches into our software and to develop custom-tailored extensions in collaborations with out clients to achieve acceptable accuracy for specific use cases.
- Understanding the client's needs: While the client's general interest was clear from the start, the specific application domain was not disclosed to us. During several occasions, we therefore could not provide an optimal solution that only became obvious at a later stage. We hope this will be limited in the near future due to a higher level of trust resulting from the long-term collaboration.
- Modelling execution: As experts in OE modelling, the most efficient way to conduct simulations as well as analyse and understand the results is to execute simulations ourselves and provide the results to the client in form of reports. Due to sensitive IP, this is not possible and lead to a large amount of support. In the future, we will overcome this barrier by providing an extended set of webinars for specific use cases. This will both increase scalability of our products and minimize training periods for the clients.
- Conquering the complexity of multiscale simulations conducted on remote resources (in-house high-performance computing (HPC) architectures or cloud resources): To obtain results in a reasonable computation time, most of our models require execution on scalable resources (~100 cores in parallel). Furthermore, results between individual modules need to be converted and copied by hand before starting each simulation step, limiting the scalability and thereby the impact of modelling. This demands a certain level of specialized expertise in HPC handling, operating systems, command line and scripting. While the client in this use case already provided this know-how from the start, this is a limiting factor for other potential customers. We therefore developed the workflow platform SimStack (www.simstack.eu) that automatically handles the information transfer and execution on remote computational resources as well as the integration of any modules into seamless workflows.