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Challenges in the Translation of materials modeling techniques to industry

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Computer simulations are a well established tool in R&D in a variety of industries, such as the automotive or aerospace industry, where virtual twins of products are developed and optimized before building the first real-world prototype. In the materials market, the application of materials modeling techniques has the potential to boost innovation by saving time and money in the development phase, and allow for shorter time to market. Modeling can aid the development process e. g. by efficient screening of variables in product design, such as materials, material combinations or process parameters, or alternatively serve as artificial microscope, delivering insights that may not, or only with great difficulty, be accessed in real experiments. This allows straight forward identification of bottlenecks in the computer and enables targeted research. Further, the incorporation of advanced and functional materials into the full virtual product design cycle, facilitated by connecting atomistic models for microscopic properties on the nanoscale to continuum models, opens up the prospect of a new level of design opportunities.

While there is a multitude of software tools and packages available with more constantly being developed and scalable computational resources are becoming gradually cheaper and more readily available, the application of materials modeling techniques often remains an academic endeavor. The uptake of these methods by industry is progressing slowly, with industrial R&D relying mostly on experimental trial&error approaches. The question how to overcome barriers limiting the application of materials modeling techniques by industry and how guide this Translation process is currently being addressed in research programs such as the H2020.

In this presentation, we elaborate on obstacles we encountered in the marketing of predictive modeling tools for Organic Electronics. These obstacles range from lack of awareness and general skepticism towards modeling to technical barriers such as handling and model accuracy. We especially highlight the bottleneck induced by the multiscale, multiphysics nature of predictive solutions. These multiscale solutions require the combination of multiple modules into workflows on a case-to-case basis, leading to a high level of technical complexity that often exceeds the expertise available in industrial R&D (especially for SMEs) and further requires specialized personnel along with extensive training periods. Ultimately, this eliminates the advantage of modeling over experiments. We show how we overcame this obstacle using a generic software platform, where academic command-line modules are incorporated and connected into market-ready workflows within a day, to be transferred to industrial end-users in form of easy-to-use desktop applications.