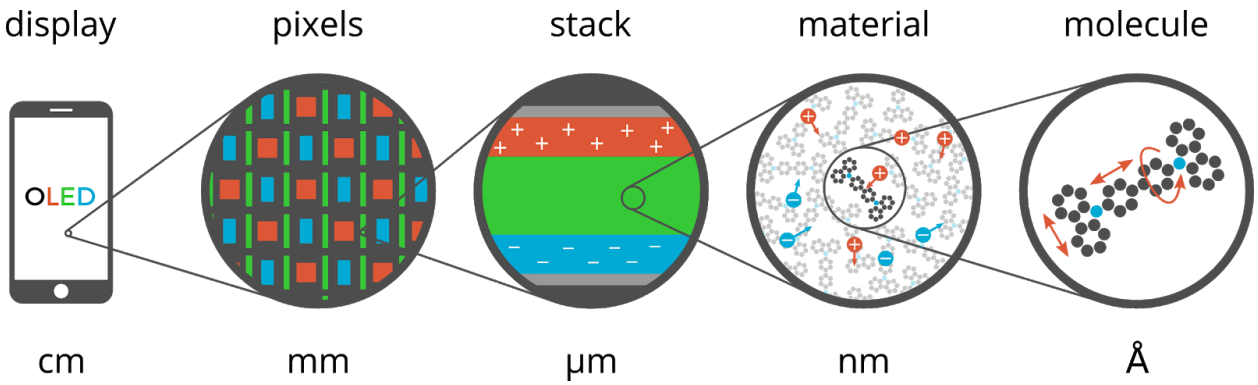
Simbeyond and Software for Chemistry & Materials (SCM) are proud to announce their collaboration on *Multiscale simulation for Organic Light Emitting Diodes (OLEDs): from molecule to device*. This project will be carried out with the support of the Dutch agency for enterprises, RVO (Rijksdienst voor Ondernemend Nederland), via the MIT R&D instrument. Starting in January 2020 this collaboration will develop the first fully integrated multi-scale simulation pipeline for OLEDs combining the years-long expertise of two Dutch companies leaders in organic device and atomistic simulation software for scientific applications in industrial and academic environments.

Modelling-based innovation is hindered by the lack of user-friendly, reliable tools that don't require costly and time-consuming training. We plan to overcome such barrier providing researchers with a robust, easy-to-use solution that doesn't require high levels of expertise from modellers, nor the cumbersome combination of several codes.



With such an integrated toolchain, users will be able to predict the performance of any combination of materials and stack architectures, under a wide range of operational conditions.

This project will streamline such quantum chemical predictions from SCM's modeling suite to serve directly as input for Simbeyond's Bumblebee software. By reducing human and computational overhead as well as improving accuracy, the digital screening and prediction of successful OLED materials and devices will be vastly accelerated.

About SCM

SCM's core activities are related to Density Functional Theory (DFT) of molecules and periodic structures (SCM has pioneered DFT in chemistry in the 1970s through the molecular DFT code ADF). Its scientific areas of expertise include spectroscopic properties in molecules and solids, all-electron basis sets throughout the periodic table, relativistic

effects including spin-orbit coupling, methods beyond DFT, DFTB and TD-DFTB, force field-based schemes such as ReaxFF, hybrid methods, and advanced embedding and solvation methods. In recent years the company has been broadening its scope beyond DFT, towards approximate, faster methods, capable of dealing with longer time scales and larger systems: the Amsterdam Modeling Suite (AMS).

About Simbeyond

Simbeyond's state-of-the-art kinetic Monte Carlo simulation code, Bumblebee, is optimized for molecular-scale simulations of opto-electronic processes in disordered systems, such as OLEDs, OPV and OFETs. Bumblebee enables the simulation of the interplay between all electronic and excitonic processes in OLEDs, at the molecular scale, in all three dimensions, and from the nanosecond timescale to the full device lifetime. The simulations predict the electrical characteristics, efficiency, color point, and lifetime of devices, based on physically meaningful material parameters, which may be obtained either from experimental data or from calculations.

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