Computer Aided Design of OLED Materials – multi-scale modeling

Software for Chemistry & Materials[1] + Simbeyond[2]

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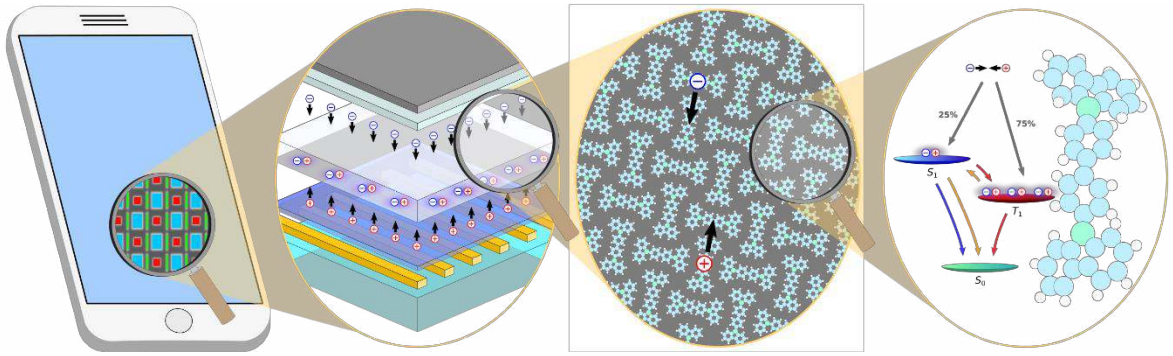
The behavior of materials, components, and therefore entire devices are ultimately determined at an atomistic level. Computational modeling can be used to predict and understand the properties of materials from an atomistic bottom-up approach. Through insight and predictive calculations the most suitable materials for a certain purpose can be selected from a large pool of candidates, reducing the time and resources to develop new and better polymers, batteries, computer chips, and organic electronic devices.

We demonstrate how industry has been using quantum chemistry to model charge transport[1,2] and luminescence properties[3,4] to predict and optimize new OLED materials. On the other end of the simulation scale, simulations of optoelectronic processes in disordered materials are necessary to predict the electrical characteristics, efficiency, color point, and lifetime of full devices[5],[6]. A brand-new collaboration between SCM and Simbeyond will develop the first fully integrated multi-scale simulation pipeline for OLEDs, marrying the Amsterdam Modeling Suite with Bumblebee. Such a user-friendly modeling platform will further reduce the development costs for new and improved OLEDs.



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