MULTISCALE MATERIAL MODELLING ON HIGH PERFORMANCE COMPUTER ARCHITECTURES

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With the accelerating materials development cycles, the development of simulation approaches for predictive, de-novo characterization and optimization of materials and device properties emerges as a grand challenge. A unified multi-disciplinary approach towards the deployment of models, tools, algorithms and simulation and visualization techniques is required to transform isolated solutions for specific problems into comprehensive, industry-ready platforms, which are capable of predicting the properties of complex materials on the basis of their constitutive elements. While many techniques exist to address the specific questions, a lack of integration of the existing methods into readily available multi-scale modelling platforms has to date limited the impact of materials-modelling techniques in materials design.

Our concept will be illustrated for one application, modelling of charge transport through organic light emitting diodes (see Figure 1), in order to demonstrate the strengths of our approach. At the macroscopic level, an organic light emitting diode is a multi-layer device comprising many different materials, each of which performs some key function in the device. The individual materials must be integrated into an electronics device and one should understand their properties as a whole in order to optimize charge transport and light emission. That is, device performance is a characteristic property not of an individual component but of the whole system, and can be described by a set of partial differential equations governing charge transport and recombination. The parameters of these partial differential equations depend on the properties of the individual layers of the device, the nature of their interfaces and even the process by which it has been assembled. All of these properties can be only understood at the quantum level, where materials simulations can be performed only for fractions of the overall device that cover less than 0.001% of its total volume.

In order to model the full device, we must therefore define a workflow which links existing simulation methods for each of the length and time scales required to treat this problem. At the lowest level this requires 100,0000s quantum calculations to characterize the hopping processes of electrons between individual molecules in a small sample of the material. The parameters gathered at this level are then fed into atomistic simulation methods, which in turn generate microscopic parameters characterizing an individual layer or an interface. The latter parameters can then be used at the continuum level to characterize the whole device. The multi-scale modeling opens new opportunity to accelerate the materials-research development cycle by in-silico experiments. It will enable virtual prescreening of OLED materials and prototype development of OLED devices in order to guide and support traditional experimentation.

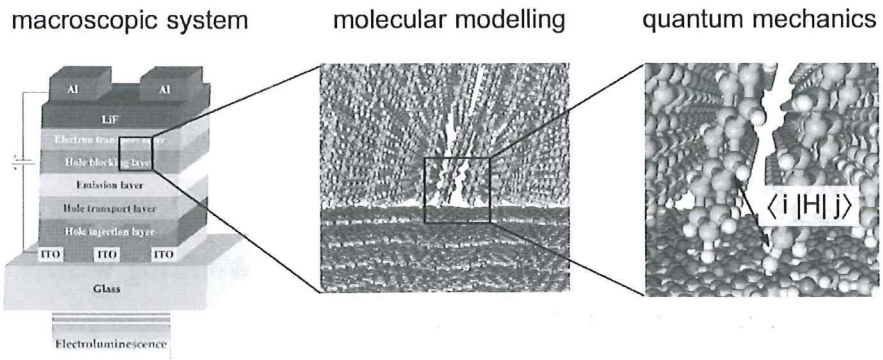

Figure 1: OLED simulations require in addition to the three scales sketched here, simulation modules to generate the morphologies and calculate charge-transport properties. A single simulation thus requires integration of five complex, but existing software solutions.