Advanced multiscale DFT simulations and beyond for complex systems

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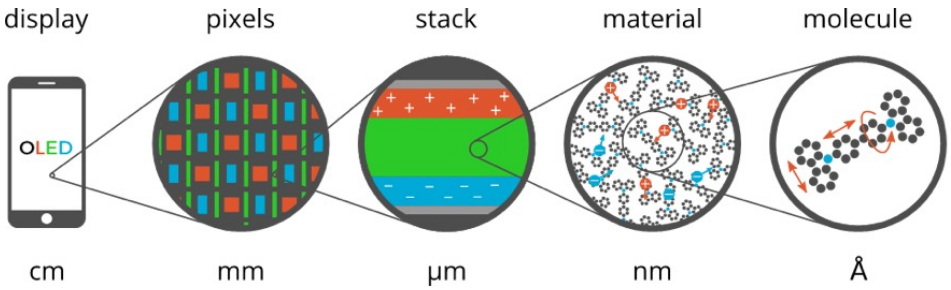
ABSTRACT

While considerable efforts have been devoted to developing precise methods for simulating either isolated molecules using ab-initio quantum chemistry techniques or larger structures using classical mechanics, the demand for accurately describing highly complex systems necessitates an integrated approach. Systems such as OLED materials have properties that are governed by intricate quantum mechanical interactions arising from numerous intermolecular forces that depend on the material's composition. To address this challenge, we have developed comprehensive workflows that enable the seamless simulation of OLED materials, leveraging cutting-edge methods encompassing both classical and quantum approaches. For the properties simulations we combine both DFT and GW [1] with polarizable embedding approaches such as the Discrete Reaction Field (DRF) [2] method to achieve a better description of the system within its real environment. The workflow comprises two primary steps: molecular component deposition and property simulation. In this presentation, we elucidate our workflow, present key findings, and unveil the latest theoretical and methodological advancements.



References

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[2] Jensen L.; van Duijnen P.T.; Snijders J.G. A discrete solvent reaction field model within density functional theory. *J. Chem. Phys.* **2003**, *118*, 514-521.