High-throughput Quantum Chemistry and Virtual Screening for Organic Semiconductor Solutions

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For the past 20 years the standard approach to drug discovery has been the automated computational screening of chemical structure libraries to identify lead systems for further investigation and experimental development. Recent advances in the power of computational resources and simulation programs have made it possible to apply this paradigm to challenges in material science. Multi-step property calculations using accurate quantum chemical methods to be executed automatically for diverse chemical libraries are now possible. Results of such calculations can then be sorted and mined to identify exemplary candidates and establish critical structure-property limits within a chemical design space. Virtual screening in which quantum chemical calculations are carried out in a high-throughput fashion to compute properties and screen for optimal materials solutions, is quickly becoming central to advanced materials chemistry research. In this presentation, use of high-throughput quantum chemistry to analyze and screen a chemical structure library is demonstrated for organic light-emitting diode (OLED) and organic photovoltaic (OPV) materials.