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High-throughout Quantum Chemistry and Virtual Screening for Materials Solutions

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Abstract – The use of virtual library enumeration and high-throughput quantum chemistry for materials discovery, analysis and optimization is introduced. Specific examples of *in silico* materials screening are presented. In particular, two illustrative cases are considered: OLED materials based on Alq3, and Li-ion battery additives based on EC. The use of Accelrys' Pipeline Pilot informatics platform for facilitating HTP modeling efforts is discussed.

The use of virtual structure libraries for computational screening to identify lead systems for further investigation has become a standard approach in drug design. Transferring this paradigm to challenges in material science is a recent possibility due to advances in the speed of computational resources and the efficiency and stability of materials modeling packages. This makes it possible for individual calculation steps to be executed in sequence comprising a high-throughput quantum chemistry workflow, in which material systems of varying structure and composition are analyzed in an automated fashion with the results collected in a growing data record. This record can then be sorted and mined to identify lead candidates and establish critical structure-property limits within a given chemical design space. To-date, only a small number of studies have been reported in which quantum chemical calculations are used in a high-throughput fashion to compute properties and screen for optimal materials solutions.[See for example Refs 1,2] However, with time high-throughput computational screening will become central to advanced materials research.

In this presentation, the use of high-throughput quantum chemistry to analyze and screen a materials structure library, representing a well defined chemical design space, is demonstrated for organic light-emitting diode (OLED) materials and Li-ion battery additives. The OLED case focuses on the chemical design space around the archetype electron-transport and emitting material tris(8-hydroxyquinoline) aluminum(III) (Alq3). The battery additive example explores the property space for derivatives of ethylene carbonate (EC).

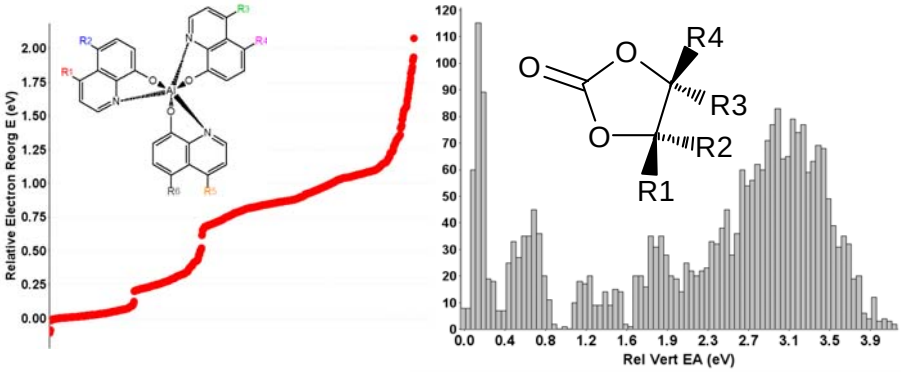

Figure 1: (Right) Electron reorganization energy computed for Alq3-based OLED materials library. (Left) Histogram of calculated electron affinities for the EC-based additive library.

References

[1] D. Morgan, G. Ceder and S. Curtarolo, Measure. Sci. Tech. 16, 296 (2005).

[2] J. Greeley, T.F. Jaramillo, J. Bonde, I. Chorkendorff and J.K. Nøskov, Nature Mater. 5, 909 (2006).