



Materials Science and Engineering: Chapter 17. Organic Photovoltaics

Carlos Amador-Bedolla, Roberto Olivares-Amaya, Johannes Hachmann, Alán Aspuru-Guzik

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Organic photovoltaics (OPVs) are particularly promising alternatives for solar-cell generation of energy because of the abundance of their constituent elements and base materials, their low cost, and relative ease of chemical synthesis; moreover, massive fabrication of related materials has been applied and constitutes an established and robust technology. The Harvard Clean Energy Project (CEP) is a high-throughput in silico screening and design effort to develop novel high-performance materials for OPVs. CEP is based on an automated, high-throughput computational infrastructure for the systematic screening of millions of OPV candidates at different levels of theoretical chemistry approaches. We have investigated the applicability of quantitative structure–property relationships (QSPR), based on descriptors of molecular properties – developed originally for drug design QSPR – in the prediction of organic monomer parameters for construction of OPVs. We developed a library of approximately 3.6 million of organic molecules, thought as promising for its use in OPVs, using a virtual reaction-based approach. We used 50 related molecules that have been studied experimentally and correlated their descriptors with their observed parameters as OPV monomers. These correlations were applied to our library of 3.6 million molecules, thus allowing us to find monomers with better merit parameters than currently known. The CEP is currently calculating theoretical chemistry properties for molecules in the library at different hierarchy levels of approximation, refining and adjusting our present findings.

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