Abstract

Small-molecule organic semiconductors are used in a wide spectrum of applications, ranging from organic light emitting diodes to organic photovoltaics. A number of factors determine their charge carrier mobility, such as molecular packing, electronic structure, dipole moment and polarizability. Presently, quantitative ab-initio models to assess the influence of these molecule-dependent properties are lacking.

Here, we present a multi-scale model, which provides an accurate prediction of experimental data over ten orders of magnitude in charge carrier mobility and demonstrate the de novo design of a novel organic semiconductor with improved mobility. The availability of first-principles based models to compute key performance characteristics of organic semiconductors may enable in-silico screening of numerous chemical compounds for the development of highly efficient opto-electronic devices.