# Understanding organics semiconductors using Density Functional Theory – hope or hopeless?

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Organic semiconductors are a scientifically fascinating and practically relevant class of materials. Hopes are high that they may contribute, e.g. in the form of organic solar cells, to solving modern societies' energy problems. Being able to theoretically understand and predict the mechanisms of light absorption, energy transfer and charge transfer in such materials can provide important guidelines, e.g., in the quest for low band gap materials that would allow for harvesting larger parts of the solar energy spectrum. However, first principles theory faces the challenge that straightforwardly solving the many-particle Schrödinger equation is close to impossible for practically relevant, large systems. Therefore, the alternative formulation of quantum mechanics that avoids the wavefunction altogether, Density Functional Theory, is frequently used for studying molecular semiconductors. However, the most commonly used density functionals fail dramatically in predicting some of the most relevant processes in organic semiconductors, such as charge transfer and transport. This talk demonstrates such failures, explains their physical origin, and argues that the problems can be eliminated without empirical input. It will be shown that recently developed, non-empirical density functionals allow for, e.g., the accurate prediction of charge transfer excitations, optical gaps, and photo-emission spectra.