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ABSTRACT

Enhancing organic solar cell efficiency: Computer simulations of materials properties

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Organic photovoltaics (OPV) are a potential, attractive sustainable energy source, however, their efficiencies are still not sufficiently high to be economically competitive. Several strategies can be employed to improve the materials for OPV, namely amongst others 1) the use of high dielectric constant materials, 2) use downconverter (singlet fission) materials, or 3) upconverter materials. Computer simulations can be used to explore the properties of materials and provide insight into the way these materials respond to perturbations, and can hence provide design guides for better OPV materials.

In this presentation on overview is given on our work on the calculation of dielectric constants for substituted fullerene derivatives. We show that we are able to predict the dielectric constants of the materials, and that we can decompose the dielectric constant into contributions from functional groups. Furthermore, we present a way to estimate singlet fission rates in organic crystals, and discuss our results obtained for potential singlet fission candidates.