

Can density functional theory predict the dielectric constant of soluble polyimides?

Introduction

<div class="df\_qntext">What is dielectric constant ()?

Dielectric constant (  $\epsilon$  ) is an important parameter affecting the power conversion efficiency of organic solar cells (OSC).

<div class="df\_qntext">Do dielectric properties affect photovoltaic efficiencies in organic solar cells?

The fill factor (FF) of organic solar cells (OSCs), a critically important photovoltaic parameter, is still sub-optimal, often less than 0.8. To further reduce the FF gaps with regard to the Shockley-Queisser upper limit, we present a study unveiling the impacts of dielectric properties on obtaining high FFs and photovoltaic efficiencies in OSCs.

<div class="df\_qntext">Can density functional theory predict the dielectric constant of soluble polyimides?

Evaluation of the insulating properties of polymers, such as the dielectric constant and dissipation factor, is crucial in electronic devices, including field-effect transistors and wireless communication applications. This study applies density functional theory (DFT) to predict the dielectric constant of soluble polyimides (SPIs).

<div class="df\_qntext">How accurate is DFT-estimated static dielectric constant?

The DFT-estimated static dielectric constant of the single-chain model accurately reproduces the corresponding experimental value with at least 80% accuracy. Our approach provides a rational and accelerated strategy to evaluate polymer insulators for electronic devices based on cost-effective DFT calculations.

<div class="df\_qntext">What is the dielectric constant of non-fullerene acceptors?

Provided by the Springer Nature SharedIt content-sharing initiative Dielectric constant of non-fullerene acceptors plays a critical role in organic solar cells in terms of exciton dissociation and charge recombination. Current acceptors feature a dielectric constant of 3-4, correlating to relatively high recombination loss.

<div class="df\_qntext">Does selenium substitution improve dielectric constant of non-fullerene acceptors?

Dielectric constant of non-fullerene acceptors plays a critical role in organic solar cells in terms of exciton dissociation and charge recombination. Here, authors report selenium substitution on central core of acceptors to improve dielectric constant, realizing devices with efficiency of 19.0%.

Our design guidelines were to bind a conventional one-dimensional thiophene-based donor molecule in a two-dimensional (2D) manner, which would lead to extended  $\pi$ -conjugation and ...

# Dielectric constant calculation of solar container density

Abstract In this study, we proposed a novel method that integrates density functional theory (DFT) with the finite field method to accurately estimate the polarizability and dielectric constant of polymers. ...

After validation of the calculation methods both on simulation and experimental values, it is shown that for a constant density, the difference between the materials could be due to the bond polarizability ...

Solcore has several ways of accessing the optical properties of materials: databases and parametric dielectric functions. Understanding the optical response of both established and novel materials is ...

A higher dielectric constant can enhance exciton dissociation and improve the overall power conversion efficiency of the solar cell. 10,000 new polymers were generated, and their ...

Solar Radiation Calculation Dr. Mohamad Kharseh E-mail: kharseh@qu.qa mohkh3@Hotmail Solar Constant is the intensity of the solar radiation hitting one square meter of the Earth

We have seen that EM radiation is a sensitive probe of the dielectric properties of materials. Absorption and reactivity experiments allow us to measure some combination of

Influences of dielectric constant and scan rate on hysteresis effect in perovskite solar cell with simulation and experimental analyses Jun-Yu Huang<sup>1</sup>, You-Wei Yang<sup>2</sup>, Wei-Hsuan Hsu<sup>2</sup>, En-Wen ...

Highlights o Fill factor improved by increasing the molecular packing density and dielectric constant o A fill factor of more than 80% and an efficiency above 18.2% OSCs were achieved o

The dielectric constant, known as the permittivity of a material, is discussed on this page. This property of a material slows down the propagation of light and reduces the wavelength. The units are Farads ...

Charge extraction techniques are a common approach to determine the charge carrier density in solar cells. 37-39 Here, the devices are ...

Physical results include the observation of previously unresolved features in the random-phase approximated dielectric function and its inverse within the framework of density ...

Donor materials with a high dielectric constant that markedly boost the efficiency have been proposed, but theoretical material designs and/or experimental results are still scarce. In this ...

Various SPIs containing trifluoromethyl groups in the backbone with different pendant types, numbers, and symmetries are successfully ...

As a case study, we perform an ab initio calculation of the dielectric constant in silicon within a popular

gradient-corrected local-density scheme. We find that the gradient corrections ...

Strategy to Calculate the Dielectric Constant of Materials 1) Start with the Hamiltonian describing the interaction of the electrons with the electromagnetic field:

In this review, we overview the current understandings on dielectric constant and its impacts on exciton dissociation and voltage losses in ...

Figure 2.6.1 : The carrier density integral. Shown are the density of states,  $g_c(E)$ , the density per unit energy,  $n(E)$ , and the probability of occupancy,  $f(E)$ . The carrier density,  $n_0$ , equals the ...

Hence, it is the time to focus on increasing the dielectric constant ( $\epsilon_r$ ) of organic materials. This review systematically summarizes the influence of  $\epsilon_r$  on OSC performance, such as ...

Dielectrics in Electric Fields - Electrical Susceptibility Naturally, one would expect the polarization of the material to be proportional to the strength of the electric field:

In particular, solar cells based on lead halide perovskites have shown great promise as evidenced by the rapid increase of the power conversion efficiency. In this ...

Overview?Note This tutorial introduces a method to calculate the thermal conductivity and viscosity of water at ambient temperature and pressure using the Green-Kubo formula. Additionally, the dielectric ...

To further reduce the FF gaps with regard to the Shockley-Queisser upper limit, we present a study unveiling the impacts of dielectric ...

Here, authors report selenium substitution on central core of acceptors to improve dielectric constant, realizing devices with efficiency of 19.0%.

We selected five typical polymers for the validation of this calculation method and found that the calculation values of IDMF-GC is roughly accurate by comparing it with the experimental ...

We report on measurement of dielectric constant, mid-gap defect density, Urbach energy of tail states in  $\text{CH}_3\text{NH}_3\text{PbI}_{1-x}\text{Cl}_x$  perovskite solar cells. Midgap defect d

In particular, solar cells based on lead halide perovskites have shown great promise as evidenced by the rapid increase of the power conversion efficiency. In this paper, we show density functional theory ...

Introduction to the manual of dielectric values The relative dielectric constant (the DC-value) of liquids and bulk solids can - next to other influencing factors - be decisive when selecting the suitable ...

## Dielectric constant calculation of solar container density

Then, the dielectric constants ( $\epsilon_r$ ) of these polymers are measured to explore their relationship with the  $E_b$ . A lack of correlation between  $\epsilon_r$  and  $E_b$  was found and therefore, suggesting that increasing the ...

High fill factor organic solar cells with increased dielectric constant and molecular packing density To further reduce the FF gaps with regard to the Shockley-Queisser upper limit, we present a study ...

The design and development of novel materials with low dielectric constants to replace traditional dielectric media, such as silicon dioxide, is an effective method to overcome the aforementioned issues.

Evaluation of the insulating properties of polymers, such as the dielectric constant and dissipation factor, is crucial in electronic devices, ...

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