

## How to Rationally Select an Interfacial Modifier for High Performance Organic Photovoltaics

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Due to low cost, flexibility, solution processing and large-scale fabrication, enormous attention is focusing on the research and development for higher OPV performance over the last decades. To improve the overall performance of organic photovoltaics, interfacial modifiers are widely applied in the device architecture to facilitate charge collection, tune the distribution of materials, and avoid pitfalls presented by traditional blocking layers such as PEDOT:PSS. Typically, interfacial layer are screened through a very laborious and empirical process that is dependent upon fabricating and testing of a large complete of devices to obtain statistically relevant data. Here, based on the surface energies of polymers and interfacial modifiers, we describe a fast and straightforward approach to enable rational selection of an interfacial modifier on device performance, prior to device fabrication. Surface energies play an integral role in device performance due to the profound influence on phase segregation within the bulk heterojunction. By simply determining the surface energies of polymers and interfacial layers, the composition of the BHJ at the interfaces could be predicted, thus enabling the user to determine the effect, positive or negative, of the interfacial layer on the device performance. Predictions were confirmed by experimental characterization and device production and testing.

**Primary authors:** YANG, Dan (Lehrstuhl für Funktionelle Materialien E 13); Dr CAO, Bing (University of Alberta, Canada); Dr HAUGER, Tate (University of Alberta, Canada); Dr LUBER, Erik J. (University of Alberta, Canada); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien); Dr BURIK, Jillian M. (University of Alberta, Canada)

**Presenter:** YANG, Dan (Lehrstuhl für Funktionelle Materialien E 13)

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