

Challenges in understanding defects in organic materials: a theorist view, focus on conjugated polymers

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Abstract

Organic conjugated polymers are a convenient choice for new electronic and optoelectronic devices, that address different goals with respect to nanotechnology: light and flexible, they can be used for large area displays and photocollectors, special transistors and others.

A sound understanding of the processes taking place on the actual device is needed, and it is hoped that theory can help as it did and does for conventional semiconductor systems. However, the systems here are much too complex and, in particular, the role of impurities and defects -coming e.g. from environmental contamination- in doping and carrier trapping is a topic very difficult to affront.

In this talk I will briefly touch on the main problems that need to be accounted for in a theoretical treatment; review recent state-of-the-art ab-initio calculations for polymer crystals, from different groups; and move on to recent results for systems with conformational defects, or chemisorbed impurities, here perforce studied through mixed theoretical formalisms.