TRR 142
Tailored Nonlinear Photonics

# TRR Guest Scientist Lecture / Seminar

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Location: Paderborn, N3.216


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## First-principles investigation of electronic properties of molecular crystals relevant to organic electronics materials


### Abstract:

For a few decades, organic molecule-based semiconductor devices, such as organic light-emitting diodes (OLEDs), organic field-effect transistors (OFETs), and organic photovoltaics (OPV), have attracted considerable attention for future flexible electronics. While some products are already on the market, and more and more developments are going on, there still remain open questions concerning the basic electronic properties of such materials, for instance about the transport mechanism of the injected charge (hole or electron). Nowadays, there are both experimental and theoretical investigations of the electronic structure of single crystals to elucidate the intrinsic electronic nature of these materials.
In this talk, I will demonstrate results of band-structure calculations for organic semiconductor crystals using the parallelized *GW* space-time code [1]. The work covers representative organic crystals: rubrene [2], picene [3], Zinc-phthalocyanine [4], oligoacenes [5], and others. I will discuss the nature of the electronic structure in terms of the crystal geometry and the intermolecular interaction, along with future plans for research during my stay at Paderborn University (09/2017–08/2018).



[1] M. M. Rieger *et al*., Comput. Phys. Commun. **117**, 211 (1999); L. Steinbeck *et al*., *ibid*. **125**, 105 (2000); C. Freysoldt *et al*., *ibid*. **176**, 1 (2007)
[2] S. Yanagisawa, Y. Morikawa, and A. Schindlmayr, Phys. Rev. B **88**, 115438 (2013)
[3] S. Yanagisawa, Y. Morikawa, and A. Schindlmayr, Jpn. J. Appl. Phys. **53**, 05FY02 (2014)
[4] S. Yanagisawa *et al*., Phys. Rev. B **90**, 245141 (2014)
[5] S. Yanagisawa and I. Hamada, J. Appl. Phys. **121**, 045501 (2017)



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