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Role of Dopant Structure and Strength in the p-Doping of Organic Semiconductors

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The p-doping of organic semiconductors (OSCs) for tuning their electronic structure in opto-electronic applications is typically done by adding strong molecular acceptors as dopants to initiate charge transfer. I will summarize the current understanding of the phenomena observed upon molecularly p-doping conjugated polymers (CPs) and molecules (COMs), where two different competing scenarios have been identified [1]: (i) integer charge transfer between OSC dopant forming ion pairs (IPAs) and (ii), fractional charge transfer, where ground-state charge transfer complexes (CPXs) between the OSC and dopant are formed. For prototypical OSCs such as poly(3-hexylthiophene) (P3HT) [2] and various oligothiophenes of different chain length [3], I will present recent findings on the role of microstructure, dopant strength, and conjugation length on the respective doping scenarios, from which chemical design strategies for improved molecular dopants emerged and are tested to suppress CPX formation [4].

[1] Salzmann et al., *Acc. Chem. Res.* 49, 370 (2016); [2] Hase et al., *J. Phys. Chem. C* 122, 25893 (2018), Hase et al., *J. Phys. Mater.* 6, 014004 (2023); [3] Liu et al., *Angew. Chem. Int. Ed.* 59, 7146 (2020); [4] Charoughchi et al., submitted.

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Keyword-2

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Keyword-3

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Primary author: Prof. SALZMANN, Ingo (Concordia University)

Presenter: Prof. SALZMANN, Ingo (Concordia University)

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