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Doping of organic and inorganic semiconductors with molecular acceptors

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Abstract

Controlled doping of semiconductors is crucial for the functionality and efficiency of modern (opto-) electronic devices. For organic semiconductors, the use of strong molecular electron donors and acceptors is meanwhile established as viable approach for doping. However, diffusion and poor thermal stability of most presently used dopants poses a challenge in applications. It turns out that the salt of the mesitylene-borinium cation (Mes_2B^+) and tetrakis(penta-fluorophenyl)borate anion $[B(C_6F_5)_4]^-$ is a superior p-type dopant for polymer semiconductors, and doping occurs *via* a charge-exchange reaction. Remarkably, the $[B(C_6F_5)_4]^-$ anion enables the stabilization of polarons *and* bipolarons in poly(3-hexylthiophene), and the effective electron affinity of $Mes_2B^+[B(C_6F_5)_4]^-$ is estimated to be 5.9 eV. The comparably high molecular weight and bulkiness of $[B(C_6F_5)_4]^-$ is expected to reduce diffusion, and no negative impact on doped polymer conductivity is observed up to 100 °C.

Notably, many of the molecular dopants used for organic semiconductors can also be employed for doping of transition metal dichalcogenides (TMDCs). When thinned to the monolayer, many are direct semiconductors, e.g., MoS_2 and WS_2, with superior optical properties. Due to the pronounced excitonic nature of TMDCs, their exciton energy and band gap depend strongly on the dielectric constant of the mechanical support used for the monolayer. Moreover, the electrical nature of the substrate plays a critical role for the mechanism by which doping with molecules occurs. Three fundamentally different charge transfer mechanisms between MoS_2 and molecular dopants have been identified and will be discussed.