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【216】 On-surface synthesis and characterization of N-doped undecacene: a combined experimental and theoretical study

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Acenes are a class of polycyclic aromatic hydrocarbons that exhibit impressive semiconductor and open-shell properties. These unique properties can be tailored to potential applications by altering the conjugated π -system with chemical doping. The synthesis of large acenes via traditional solution-chemistry route is hindered by their poor solubility and high reactivity. In this work, we present the on-surface synthesis of undecacene doped with nitrogen atoms replacing the edge carbon atoms of the third outer benzenoid rings. The N-doped undecacene is characterized by scanning tunneling and non-contact atomic force microscopy on Au(111), supported by density functional theory and GW calculations. Furthermore, we use ab initio simulations to characterize the effects of the doping to the aromaticity and open-shell properties of the system.

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