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**Complex Stoichiometry reordering of PTCDA on Ag(111) upon K Intercalation** G.P. BRIVIO, A. BABY, Univ. Milano-Bicocca (Italy), C. ZWICK, M. GRUENEWALD, R. FORKER, T. FRITZ, Univ. Jena (Germany), G. FRATESI, Univ. Milano (Italy), O.T. HOFMANN, E. ZOJER, Graz Univ. Technology (Austria) — Alkali metal atoms are a simple yet efficient n-type dopant of organic semiconductors. However, the molecular crystal structures need be controlled and well understood in order to optimize the electronic properties (charge carrier density and mobility) of the target material. Here, we report that potassium intercalation into PTCDA monolayer domains on a Ag(111) substrate induces distinct stoichiometry-dependent structural reordering processes, resulting in highly ordered and large  $K_x$ PTCDA domains. The emerging structures are analyzed by low temperature scanning tunneling microscopy (STM), scanning tunneling hydrogen microscopy (STHM), and low-energy electron diffraction (LEED) as a function of the stoichiometry and by density functional theory (DFT) calculations. Large stable monolayer domains are found for  $x=2,4$ . The epitaxy types for all intercalated stages are determined as point-on-line. The K atoms adsorb in the vicinity of the oxygen atoms of the PTCDA molecules, and their positions are determined with sub-Angstrom precision. This is a crucial prerequisite for the prospective assessment of the electronic properties of such composite films, as they depend on the mutual alignment between donor atoms and acceptor molecules.

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