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Following the molecular self-assembly on solid surfaces in real-time

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In the contribution, we will first review the principles of molecular self-assembly on solid surfaces. Then we will follow the kinetics of the deprotonation-induced irreversible phase transitions of 4,4'-biphenyl dicarboxylic acid (BDA) on Ag(001) surface under ultra-high vacuum conditions. The real-time view by low energy electron microscopy (LEEM) complemented with low energy electron diffraction (LEED), STM, non-contact AFM, and XPS, supported by DFT and kinetic Monte Carlo simulations, provides new insights on the deprotonation reaction. The phase transformation is shown to exhibit a wide variety of phenomena that are well described by a general growth-conversion-growth (GCG) model. Here, the two-dimensional gas of admolecules has a dual role: it mediates mass transport between the molecular islands and hosts a slow deprotonation reaction. We show that our observations are consistent with burst nucleation kinetics and point out the significant role of surface step-edges in this process. In the full molecular layer, the mass transport via on-surface diffusion in the full monolayer is hindered, and phases different than for the monolayer are observed.

As a separate topic, we will briefly discuss the formation of M-TCNQ (M = Fe, Ni, Mn) networks self-assembled on graphene/Ir(111). Here, all the employed metals show the same structural motif with 1:1 M:TCNQ stoichiometry. The M-TCNQ structure is present in three non-equivalent orientations on the graphene substrate. The most robust is the Fe-TCNQ network; it is thermally stable up to ca. 550 °C. In contrast, Ni-TCNQ decomposes already upon heating to 330 °C but is stable under ambient conditions.