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Self-assembly and surface-assisted reactions of halogen-containing molecules

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A combination of scanning tunneling microscopy, atomic force microscope and theoretical calculations were used to elucidate the interactions in halogen bonding driven molecular self-assemblies on metal surfaces. Distinct bonding configurations between halogen atoms were identified, whose features depend on the environments of the respective halogen atoms and substituent groups. By introducing transition metal atoms, hybrid metallo-supramolecular assemblies were constructed via coordination bonding to the halogen ligands. The spontaneously formed molecular architectures via halogen-bearing molecules enable us to further explore in-situ synthesis of graphene-related nanostructures on surfaces. We revealed the reaction pathway of a few halogen substituted aromatic molecules in an effort toward rational fabrication of carbon-based nanostructures with atomic precision.