Temperature Induced On-Surface Ring-Opening Polymerization Reaction for the Synthesis of Nanoribbons: Strain Influence of Cycloparaphenylenes

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In on-surface synthesis (OSS), many reactions are performed via an Ullmann-type reaction step, involving halogenated precursors. However, in the reaction steps, cleaved halogen adatoms might disturb the interaction of intermediates and product formation. Therefore, there is a growing demand for halogen-free precursors when performing on-surface reactions. Recently, we found that halogen-free [6]Cycloparaphenylene ([6]CPP) is suited to thermally induce a ring-opening polymerization (ROP) to synthesize graphene (GNR) and biphenylene nanoribbons (BNR) via undisturbed formation of ordered poly(*para*-phenylene) (PPP) chains. [1] However, the mechanism of this reaction and the use of CPP's as precursors in OSS is not well understood yet. In this study, we investigate the strain influence of a set of Cycloparaphenylenes of different sizes (namely [6]CPP, [8]CPP and [10]CPP). [2] Our results suggest that the ROP is facilitated when performing the ROP with smaller, highly strained CPP's such as [6]CPP. For larger CPP's with lower strain energies the initial ring opening is hampered, leading to only partial polymerization for [8]CPP and no polymerization in the case of [10]CPP. Furthermore, dehydrogenation of individual phenyl rings in intact CPP rings is observed in case of [8]CPP and [10]CPP which hinders polymerization.

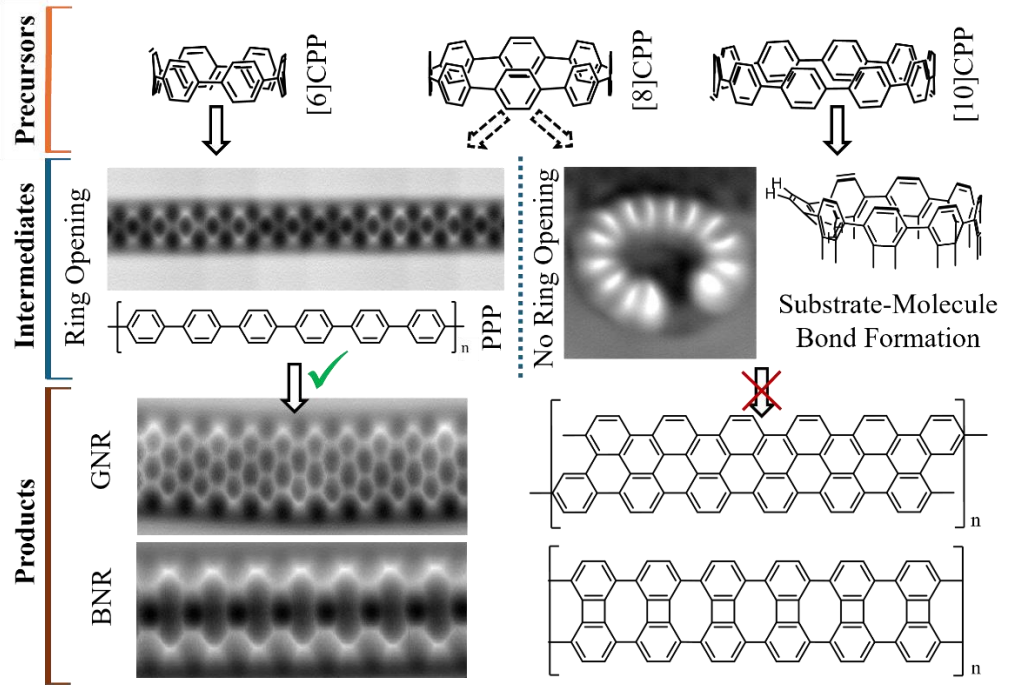

Figure 1. Reaction path of the ROP of CPP's. A full polymerization is observed for [6]CPP, whereas for [8]CPP and [10]CPP only partly or no polymerization reaction is observed.

[1] Fan and Zhong et al., Ultra-Long PPP via Strain-Induced On-Surface Ring-Opening Polymerization for Access to Nonbenzenoid Carbon Nanoribbons, *Submitted*

[2] Wiche et al., Temperature Induced On-Surface Ring-Opening Polymerization Reaction for the Synthesis of Nanoribbons: Strain Influence of Cycloparaphenylenes, *In Preparation*