

Designing Organic π -Conjugated Molecules for Crystalline Solid Solutions: Adamantane-Substituted Naphthalenes

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We showcase herein organic crystalline solid solutions (CSSs)^[1-3] based on the simplest polycyclic aromatic hydrocarbon (PAH) scaffold, naphthalene, stabilized by dispersion forces induced by adamantane substitution. High thermal stability of the host and guest molecules synthesized by cross-coupling of dibromonaphthalene derivatives and 4-(1-adamantyl)phenyl boronic ester enabled formation of crystals by sublimation. We could generate binary monocrystalline solid solution systems proven by X-ray crystallography, the first system of designed CSSs stabilized exclusively via dispersion forces with structural evidence. These observations are additionally supported by lattice energy calculations and spectroscopic examinations.^[4]

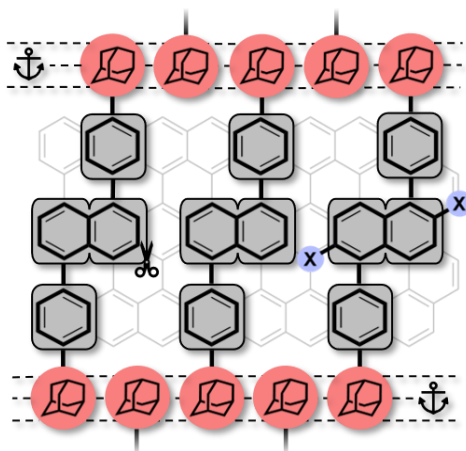


Figure 1: A schematic drawing of the design principle for PAHs with adamantane substituents.

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