Supramolecular studies of perylenediimide tetrahedral cages

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Perylenediimides (PDIs) are a class of organic semiconductors which exhibit high thermal, chemical and photochemical stability. Mesityl-substituted PDI (mes-PDI) exists in two crystalline polymorphs, one of which comprises π-stacked dimers.[1] In this structure, each isolated dimer is surrounded by a solvent void (Figure 1). These dimers assemble into tetrahedral cages which are held together exclusively through non-covalent interactions, namely the π–π stacking of perylene cores and CH··π interactions of the mesityl rings. This talk will discuss variable temperature studies of these cages, illustrating their excellent thermal stability.

Additionally, time-correlated single photon counting experiments show different photophysical characteristics for each polymorph. Further “pump-and-probe” photophysical studies are being undertaken at the Photon Factory (Japan) and involve time-resolved excited-state crystallographic studies of the mes-PDI cages upon irradiation.

![Figure 1](image.png)

**Figure 1.** Two tetrahedral cages of mes-PDI, illustrating a π-stacked dimer, surrounded by a solvent void.


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