Supramolecular Engineering of Functional Materials

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For a period of more than twenty years our group has studied the formation of molecular aggregates and the functional properties originating from the interaction of various π-systems (merocyanines, squaraines, polycyclic aromatic imides) in terms of structure-function relationships. Dimers were of particular value because they can be synthesized easily and with their still modest size can be elucidated by higher level quantum chemical methods. In this lecture I will showcase perylene bisimides (PBIs), a class of materials characterized by a particularly rich functional complexity, originating from strong structure-dependent electronic couplings between the molecular building blocks. Thus, with a knowledge-based supramolecular engineering approach PBI-based molecular aggregates and materials can be engineered that exhibit desirable properties for a variety of applications from traditional colorants up to solid state emission and organic electronics.

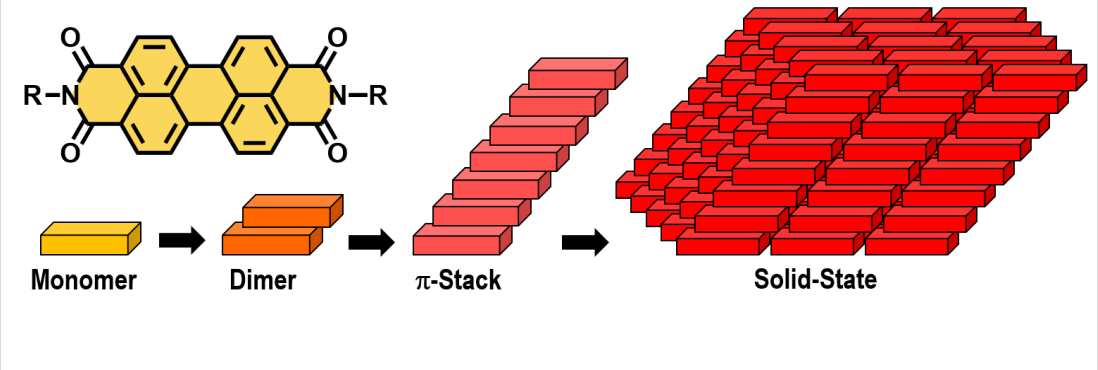

Figure 1: Molecular matter from monomers via aggregates up to solid state materials.

References:

[1] R. K. Dubey, F. Würthner, *Nat. Chem.* **2023**, *15*, 884: Playing Lego with perylene dyes

[2] F. Würthner, C. R. Saha-Möller, B. Fimmel, S. Ogi, P. Leowanawat, D. Schmidt, *Chem. Rev.* **2016**, *116*, 962–1052: Perylene Bisimide Dye Assemblies as Archetype Functional Supramolecular Materials