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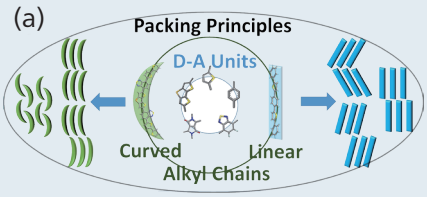
Packing Principles for Donor-Acceptor Conjugated Molecules

Simple packing principles are found in lattices of structurally complicated D-A conjugated molecules.

Donor-acceptor (D-A) conjugated molecules have been the main character in the development of organic optoelectronics for the past 15 years. Above the length scale of a molecule, the solid-state morphology acts as an important intermedium to transfer molecular properties into useful device performance. Although synthetic chemistry of D-A molecules has been vigorously developed, the key factors that affect the assembly behavior and the lattice structures of D-A molecules have been only sparsely discussed.

D-A molecules require accessible thermodynamic and kinetic paths to assemble into an ordered solid-state structure. According to the Hunter-Sander principle, aromatic units in the edge-to-face or displaced face-to-face arrangements have favorable π-π interaction. As a result, conjugated molecules typically have a thermodynamic driving force to assemble into ordered phases. Nevertheless, D-A molecules are complicated in their chemical structures, because the molecules possess a (linear or curved) conjugated backbone, terminal substituents and lateral substituents. The easily distorted geometry of the conjugated backbone and the incommensurate packing dimensions of the backbone and the substituents make the assembled structure not only unpredictable but also kinetically difficult for the D-A molecules to assemble.

Chien-Lung Wang, Wei-Tsung Chuang and their colleagues at National Chiao Tung University and NSRRC, summarized more than 40 crystal lattices of conjugated oligomers to identify the packing principles for D-A conjugated molecules[1,2]. By analyzing the packing models of the conjugated molecules in the crystal lattices, the morphological influences of the backbone curvature, terminal substituents and lateral substituents of D-A molecules were revealed as illustrated in **Fig. 1(a)**. Important packing models including a perpendicular arrangement and a tilted arrangement were identified from the lattices of the conjugated molecules with straight backbones, whereas scaly packing and intercalated packing were found in the lattices of those with curved backbones. In addition to the backbone curvature, terminal substituents were observed to influence the tilt angle of conjugated molecules in the plane of the tilted arrangement. Notably, because the lateral substituents prevent edge-to-face packing of the backbones, the (brick wall or staircase) face-to-face π-stacking was found in crystals of the laterally substituted conjugated molecules.



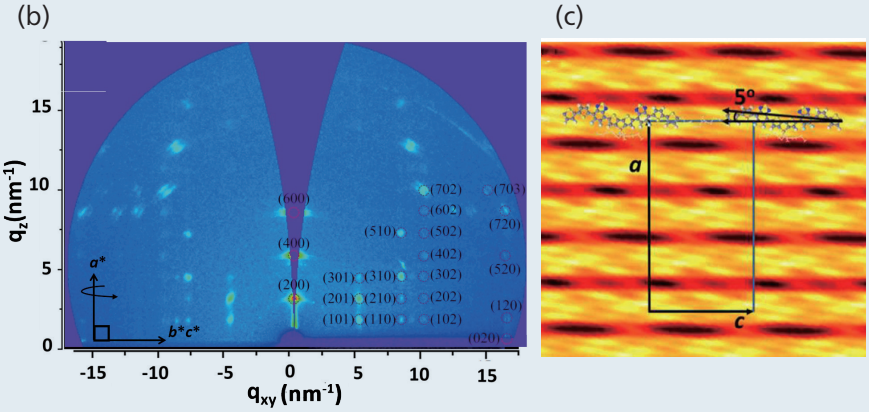
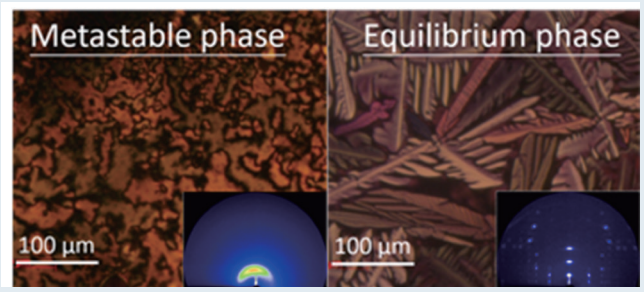


Fig. 1: (a) Packing principles of D-A conjugated molecules. (b) GI-XRD. (c) Electron density map of a DTS-F_2BT D-A molecule. [Reproduced from Ref. 1 and 2]

Through scrutiny of the lattices, packing disorder was also found in the lattices of D-A molecules. The presence of disorder in the lattices implies that attaining a total long-range solid-state order is difficult for D-A molecules that are structurally complicated and readily distorted. When applied to optoelectronics in particular, a short processing time increases the possibility of forming thin films of D-A molecules with structural disorder. To identify the exact thin-film morphology of D-A oligomers, they further undertook a in situ GI-XRD experiment to identify the phase development of a DTS-F_2BT D-A molecule, and developed techniques to transfer the information in the GI-XRD pattern (**Fig. 1(b)**) into a real-space packing model of the molecule (**Fig. 1(c)**). So far, the phase behavior of D-A molecules in the formation of active thin films remains difficult to comprehend. The work of Chuang and Wang represents an important step forward in the continuous advances in methods of characterization to attain a true structure-property relation of D-A molecules in optoelectronic applications. (Reported by Chien-Lung Wang, National Chiao Tung University)



This report features the work of Chien-Lung Wang, Wei-Tsung Chuang and the colleagues at National Chiao Tung University and NSRRC published in Chem. Mater. ***28****, 5175 (2016) and Chem. Mater.* ***28****, 8980 (2016).*

TLS 01C2 SWLS – X-ray Powder Diffraction
TLS 17A1 W200 – X-ray Powder Diffraction
TLS 13A1 SW60 – X-ray Scattering
TLS 23A1 IASW – Small/Wide Angle X-ray Scattering

- X-ray Diffraction, Grazing-incidence X-ray Scattering, High/Low-temperature Phase Transition, Solution and Thin Film Characterization
- Materials Science, Chemistry, Condensed-matter Physics, Soft Matter, Alloy and Inorganic Chemistry, Polymer Science

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Elucidating the DNA-Histone Interaction in a Nucleosome from the DNA-Dendrimer Complex

Using a DNA-dendrimer complex as a model system, synchrotron small-angle X-ray scattering revealed that the interaction between DNA and the histone protein in a nucleosome is beyond electrostatics, as additional specific interactions must exist to fix the DNA superhelix around histone and to select the favored DNA sequence to form the nucleosome core particle.

The genome of eukaryotic organisms contains many genetic codes carried by DNA. The longest DNA in a chromosome can extend to as much as 2 m in a fully stretched length. As the cell nucleus in which the chromosomal DNA is accommodated has dimension about 10 μm, the long DNA chains must be hierarchically compacted with several levels to fit into the limited space of the nucleus. This problem, known as chromatin folding, is still under intensive study, as the detailed hierarchical structure associated with the DNA compaction has not been resolved completely.[1] Chromatin is composed of a basic building block called a nucleosome core particle (NCP), which is interconnected by the linking DNA to form the so-called beads-on-string (BOS) structure. NCP contains a histone octamer (HO) and the nucleosomal DNA (~147 bp) that wraps around the HO with a left-handed 1.75 turn superhelix of which the pitch length is 25.6 Å. According to the intrinsic charges of DNA and HO, NCP can be regarded as an electrostatic complex of a