

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 an in situ GI-XRD experiment to identify the phase development of a DTS-F₂BT 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 applica-

tions. (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

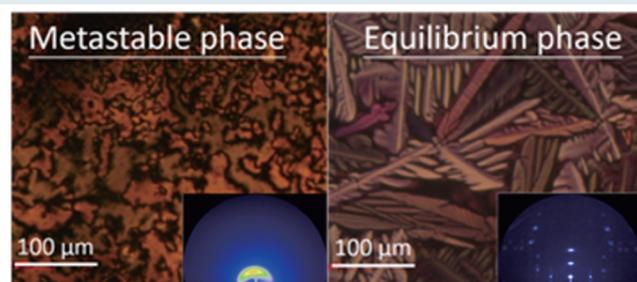
TLS 13A1 SW60 – X-ray Scattering

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

DNA polyanion and a HO macrocation. Using an electrostatic complex of DNA with poly(amidoamine) (PAMAM) G6 dendrimer (called dendriplex) as a model system, a research team led by Hsin-Lung Chen (National Tsing Hua University) has resolved that the attractive interaction between DNA and HO is beyond electrostatics. This conclusion was formed on comparing the key structural features of the dendriplex with those of the nucleosome array revealed by synchrotron small-angle X-ray scattering (SAXS) at **TLS 23A1**.²

Dendrimers are a tree-like hyperbranched macromolecule of a unique type with perfectly symmetric branching beginning from a central core. PAMAM G6 dendrimer of diameter ca. 67 Å is geometrically similar to HO. When one-third of the amine groups are protonated, PAMAM G6 dendrimer carries approximately the same charge as HO; the complex of this specific dendrimer with DNA might hence serve as a simplified model system to facilitate an understanding of the fundamental problems associated with chromatin, including DNA-HO interaction, linking DNA formation, and chromatin folding.^{3,4}

In the first part of this work, the authors investigated the structure of the dendriplex formed through a pure electrostatic interaction between DNA and PAMAM G6 dendrimer. They found that DNA was able to wrap onto the dendrimer to form the BOS structure, of which the pitch was comparable with that in the nucleosome. The wrapping trajectory in the dendriplex system was, however, loose and fluctuating; the distance between adjacent beads (the DNA-wrapped dendrimer) was near the diameter of a single PAMAM G6 dendrimer, indicating that the linking DNA between the beads was short, as shown in **Fig. 1**.

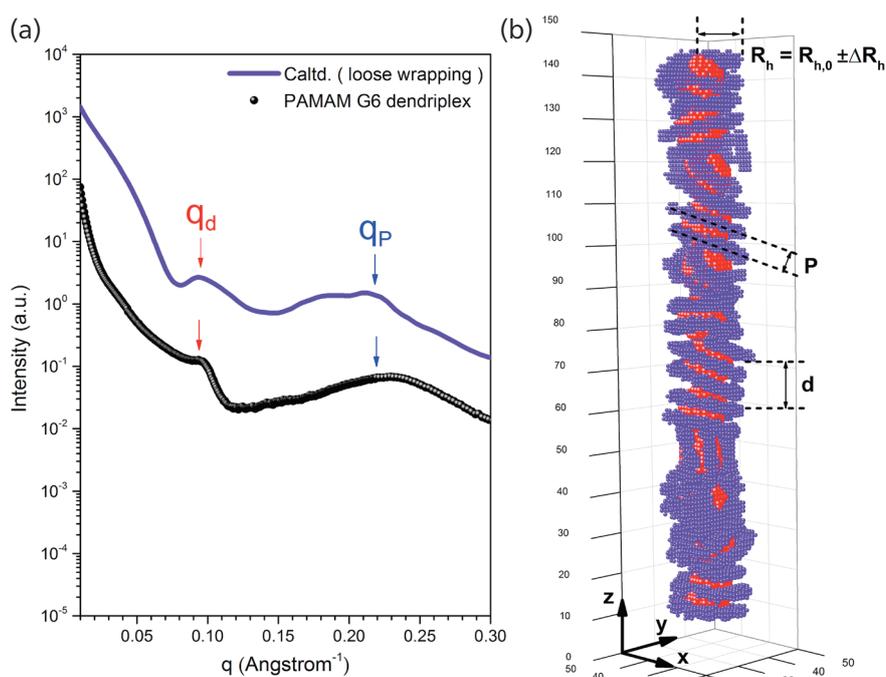


Fig. 1: (a) Calculated and experimental SAXS profiles of PAMAM G6 dendriplex. q_d and q_P denote characteristic scattering vectors associated with the interparticle distance between the beads and the pitch length of the DNA superhelix, respectively. (b) Coarse-grain model of the BOS structure of PAMAM G6 dendriplex. P and d denote the pitch length of DNA superhelical trajectory and the interparticle distance between the beads, respectively. R_h is the local radius of the DNA superhelix. [Reproduced from Ref. 2]

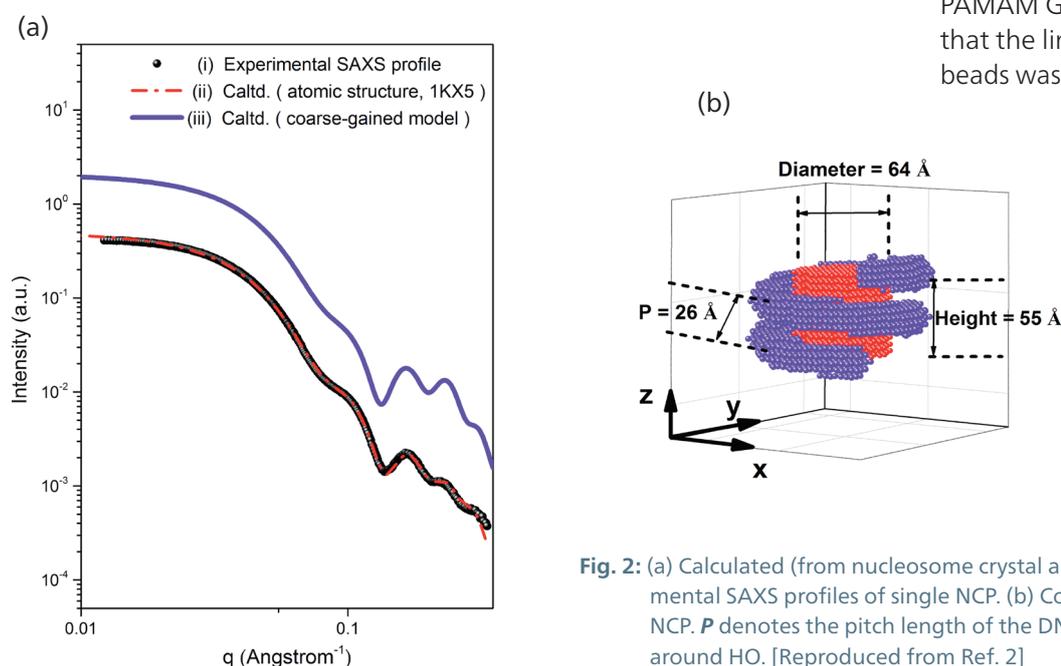


Fig. 2: (a) Calculated (from nucleosome crystal and coarse model) and experimental SAXS profiles of single NCP. (b) Coarse-grain model of single NCP. P denotes the pitch length of the DNA superhelix wrapping around HO. [Reproduced from Ref. 2]

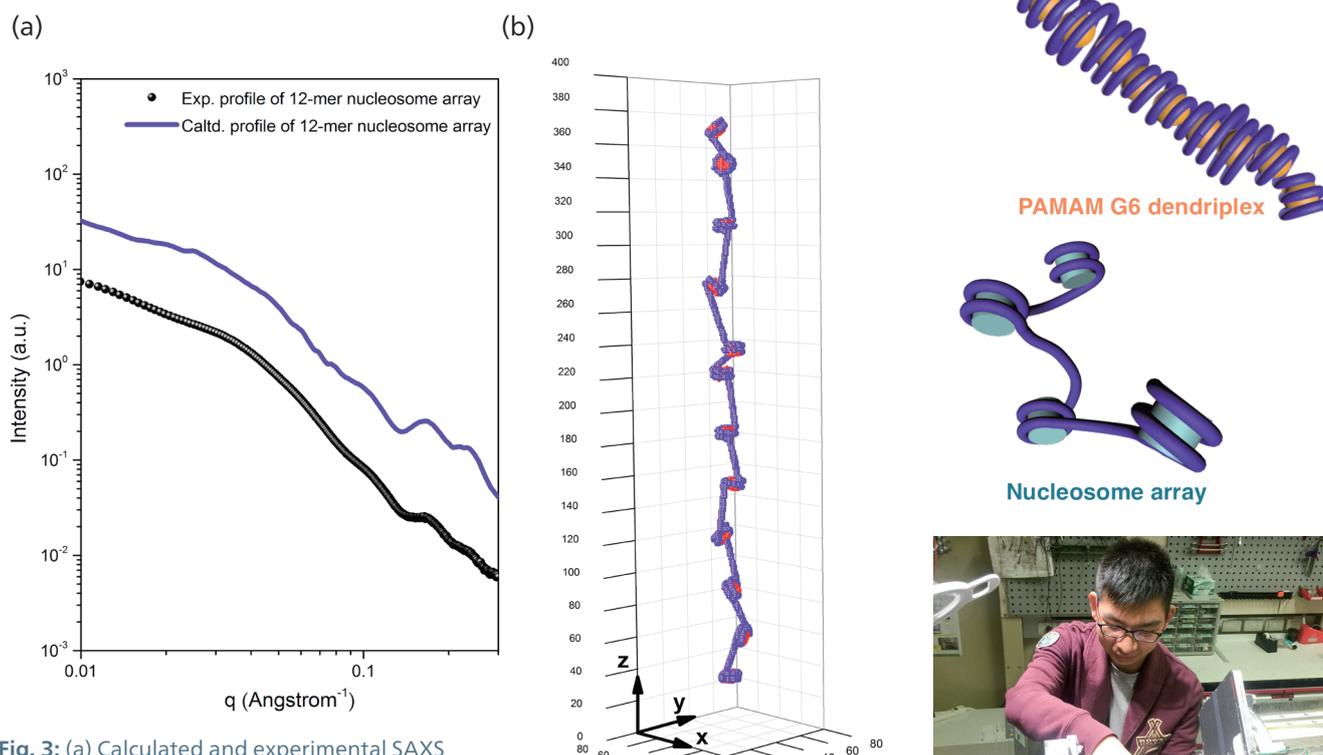
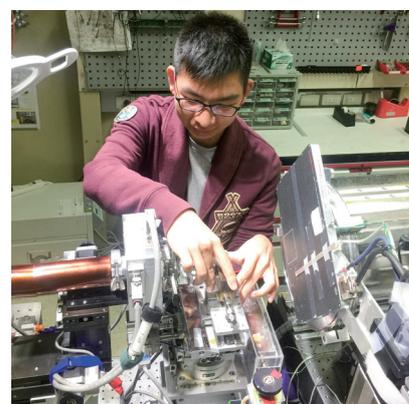


Fig. 3: (a) Calculated and experimental SAXS profiles of 12-mer nucleosome array. (b) Coarse-grain model of 12-mer nucleosome array used to calculate the SAXS profile. [Reproduced from Ref. 2].



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Chen's group proceeded further to resolve the structures of NCP and the 12-mer nucleosome array prepared by Lars Nordenskiöld's group at Nanyang Technological University, Singapore. The SAXS profile of NCP was found to agree satisfactorily with that calculated from the crystal structure of NCP, indicating that DNA wraps around HO through a sustained trajectory with limited fluctuations (Fig. 2). The global conformation of the 12-mer nucleosome array was eventually identified through a comparison of the experimental SAXS profile with that calculated from the coarse-grain model. The result demonstrates that the NCP in the array were well separated with a long linking DNA, as shown in Fig. 3.

This work has thus disclosed that both dendrimer and HO have the ability to attract a DNA chain to wrap around them with a comparable pitch length, but the wrapping trajectory in the dendriplex system in which only the electrostatic interaction is operative is loose and fluctuating, whereas DNA wraps around HO through a sustained trajectory with limited fluctuations. Furthermore, the dendrimers in the dendriplexes were gathered closely by DNA to achieve a minimum Gibbs energy by means of overcharging, whereas the NCP in the nucleosome array were well separated with a long linking DNA. The results indicate the existence of additional specific interactions beyond electrostatics between HO and

DNA in nature to fix the DNA superhelix around HO and to select the favored DNA sequence to form the NCP. (Reported by Yen-Chih Huang, National Tsing Hua University)

This report features the work of Hsin-Lung Chen and his collaborators published in Macromolecules **49**, 4277 (2016).

TLS 23A1 IASW – Small/Wide Angle X-ray Scattering

- SAXS
- Materials Science, Soft Matter

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