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Molecular Packing Details of Photocatalytic Perylene Amphiphile Nanosheets via X-ray Scattering[1] BORIS HARUTYUNYAN, ADAM DANNENHOFFER, SUMIT KEWALRAMANI, TANER AYTUN, DANIEL FAIRFIELD, SAMUEL STUPP, MICHAEL BEDZYK, Northwestern Univ, ARGONNE-NORTHWESTERN SOLAR ENERGY RESEARCH CENTER COLLABORATION — Molecular packing in light harvesting 2D assemblies of photocatalytic materials is a critical factor for solar-to-fuel conversion efficiency. However, the structure-function correlations have not yet been fully established. This is partly because of the difficulties in extracting the molecular arrangements from the complex 3D powder averaged diffraction patterns of 2D lattices, obtained via in-situ wide-angle X-ray scattering. Here, we develop a scattering theory formalism and couple it with simple geometrical model for the molecular shape of chromophore 9-methoxy-PMI (MeO-PMI) used in our study. This generally applicable method fully reproduces the measured diffraction pattern including the asymmetric line-shapes for the Bragg reflections and yields the molecular packing arrangement within a 2D crystal with a remarkable degree of detail. We find an approximate edge-centered herringbone structure for the PMI fused aromatic rings and ordering of the chains. This packing arrangement differs from the more symmetric face-to-face orientation of the unsubstituted PMI rings, which is correlated to our measurement of the reduced catalytic performance of MeO-PMI nanosheets as compared to the mesoscopically similar unsubstituted PMI assemblies.

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