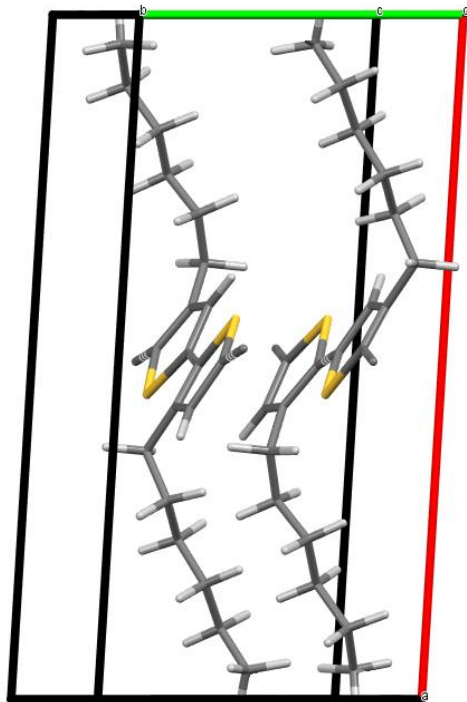


Resonant X-ray Diffraction Reveals Backbone Tilt in Polymers



Molecular packing of the polymer poly(3-hexylthiophene)

G. Freychet, P. Chantler, Y. Huang, W. Liang Tan, M. Zhernenkov, N. Nayak, A. Kumar, P. A. Gilhooly-Finn, C. B. Nielsen, L. Thomsen, S. Roychoudhury, H. Siringhaus, D. Prendergast, C. R. McNeill. *Materials Horizons*. **9** (6), 1649-1657 (2022).

This work was performed at the National Synchrotron Light Source II (NSLS-II) and the Molecular Foundry.

National Synchrotron Light Source II

Scientific Achievement

By employing resonant tender x-ray diffraction, scientists resolved the tilt of the backbone of a conjugated polymer, an important structural feature that is otherwise hard to discern with other research tools and has eluded measurement.

Significance and Impact

Conjugated polymers, due to their unique electronic and optical properties, have applications in solar cells and electronics; however, scientists have a hard time pinning down the precise molecular alignment in these polymers and its expected relationship to optimal properties.

Research Details

- Studied the backbone tilt of crystalline poly(3-hexylthiophene) at the SMI beamline at NSLS-II using resonant tender x-ray diffraction.
- Determined a 30 ± 5 degrees tilt of the backbone with respect to the side chain stacking direction (a axis of the unit cell).

