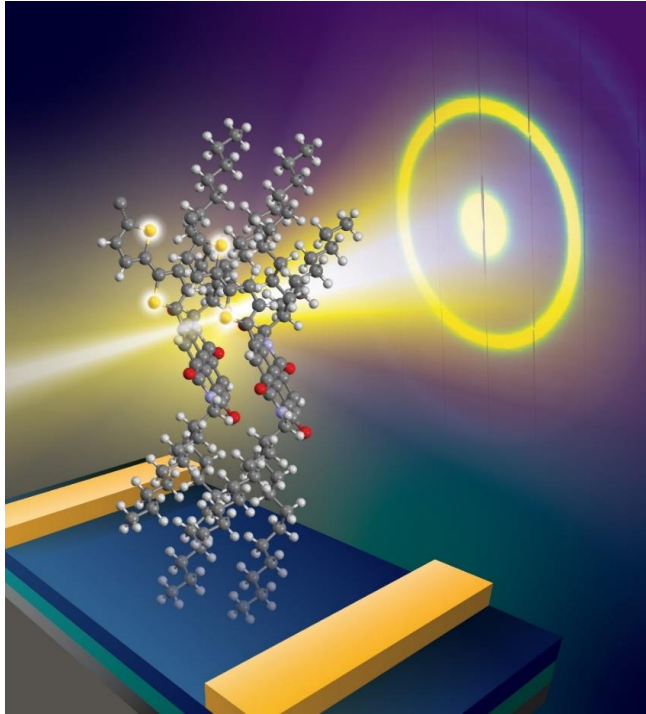


# New Way of Revealing Molecular Packing



*The image shows X-rays resonating with sulfur atoms in the polymer that gives extra information in the X-ray diffraction pattern.*

G. Freychet, E. Gann, L. Thomsen, X. Jiao, C. R. McNeill. *J. Am. Chem. Soc.* 143 (3), 1409-1415 (2021).

*Work was performed in part at Brookhaven National Laboratory*

## Scientific Achievement

Scientists demonstrated a new approach using resonant tender x-ray diffraction to reveal the details of the molecular packing in polymers containing sulfur.

## Significance and Impact

Polymers are hard to study with x-ray diffraction as they are disordered and interact weakly with x-rays. Tuning the wavelength so that the x-rays resonate with sulfur atoms allows new information about their microstructure to be unlocked, aiding the development of devices based on semiconducting polymers.

## Research Details

- Investigated a polymer using resonant tender x-ray diffraction at the SMI beamline at NSLS-II.
- Revealed changes of the resonant diffraction intensity based on polymer packing arrangements.
- Calculated the resonant different polymer packing motifs and compared them with measured diffraction signal to determine the packing in the sample.