



Contribution ID: 45

Type: Oral

Scattering or spectroscopy? Both!

Thursday, 25 November 2021 13:30 (20 minutes)

In this presentation I will discuss the development of resonant tender X-ray diffraction to study the molecular packing of semiconducting polymers. Semiconducting polymers are being developed for application in a wide range of optoelectronic devices including solar cells, LED and transistors. Being polymeric materials they offer advantages over traditional semiconductors including ease of processing and mechanical flexibility. Most semiconducting polymers are semicrystalline, with the way in which polymer chains pack strongly affecting their optoelectronic performance. Unlike small molecule crystals whose structure can be directly solved using crystallographic methods, semiconducting polymers are more disordered meaning that there are not enough diffraction peaks available. To squeeze more information from the diffraction peaks that are present, we have turned to resonant diffraction: By varying the X-ray energy across an elemental absorption edge, the variations in diffraction intensity that are observed can provide additional information. Also known as anomalous diffraction this technique has been applied in other fields including protein crystallography. As many semiconducting polymers utilise sulfur as heteroatoms, we have studied resonant diffraction effects at the sulfur K-edge in the tender X-ray regime. Furthermore we have adopted a spectroscopic approach exploiting anisotropic near-edge X-ray absorption features at the sulfur K-edge that produce highly anisotropic resonant diffraction effects. This marrying of spectroscopy and scattering enables us not only to infer information about the position of the resonant atoms within the unit cell, but also to deduce the orientation of molecular bonds and orbitals within the unit cell.

Presenter Gender

Man

Do you wish to take part in the Student Poster Slam

Condition of submission

Yes

Students Only - Are you interested in AINSE student funding

Level of Expertise

Expert

Pronouns

Which facility did you use for your research

Australian Synchrotron

Primary author: Prof. MCNEILL, Chris (Monash University)

Presenter: Prof. MCNEILL, Chris (Monash University)

Session Classification: Physics, Surface & Condensed Matter

Track Classification: Physics, Surface & Condensed Matter