Fakultät für Naturwissenschaften

Institut für Chemie und Institut für Physik

GDCh
Gesellschaft Deutscher Chemiker

laden ein

gemeinsam mit der Gesellschaft Deutscher Chemiker zum

Vortrag
von Herrn

Prof. Christopher McNeill

Department of Materials Science and Engineering
Monash University
Clayton/Australien

“Resonant Tender X-ray Scattering of Conjugated Polymers”

am: 16. November 2023

um: 16:00 Uhr

wo: im Raum 1/232

Die kleine Kaffeerunde vor dem Vortrag beginnt um 15:30 Uhr im Raum 1/232. Das Mitbringen von eigenen Trinkgefäßen ist erwünscht.

TECHNISCHE UNIVERSITÄT
IN DER KULTURHAUPTSTADT EUROPAS
CHEMNITZ

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“Resonant Tender X-ray Scattering of Conjugated 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, and the way in which polymer chains pack strongly affects their optoelectronic performance. Unlike small molecule crystals whose structure can be directly solved using established 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 tender X-ray diffraction: By varying the X-ray energy across an elemental absorption edge, variations in diffraction intensity are observed that can provide additional information about molecular packing. Also known as anomalous diffraction, this technique has been applied in other fields such as 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. By performing high resolution energy scans across the sulfur K-edge, we show that spectroscopic information relating to specific bonds and molecular orientation can be discerned in the resonant X-ray diffraction profiles. Indeed, by understanding the anisotropic X-ray absorption properties of these materials we are able to interpret this data allowing us to distinguish between different crystalline polymorphs and resolve the tilting of the polymer backbone with respect to the unit cell axes. In general our work highlights how the fields of crystallography and spectroscopy can be combined to provide new insights into the molecular packing of weakly ordered soft materials.

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