

Resonant Tender X-ray Scattering and Diffraction: a key tool to reveal the location of counterions in polymeric organic mixed ionic/electronic conductors

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Resonant x-ray scattering and diffraction is an emerging technique for the nanostructure characterization of soft matter. While these approaches are widely spread for highly ordered material, the amorphous or paracrystalline nature of most of the soft matter systems limits the use of currently developed method such as diffraction anomalous fine structure technique.

In this presentation, we will illustrate the use of resonant x-ray scattering on conjugated polymers used for optoelectronic devices [1, 2]. The performance of such devices are highly dependent upon the molecular packing however. The presence of sulfur atoms in common conjugated polymer such as P3HT or N2200 enable the use of tender x-rays (sulfur K-edge is around 2.47 keV) to probe and enhance signals from the sulfur atoms. Tracking the intensity variation across the sulfur K-edge and comparing with theoretical calculation enable to discriminate between different packing geometries and to extract important new microstructural information. We will both present results in the transmission geometry, on thin films deposited on Si₃N₄ membranes, as well as in the grazing-incidence (GI) geometry on thin film on Si substrate. Especially for the GI geometry, we will discuss the importance of x-ray absorption and its impact/distortion on the collected signal [3].

Then, we will show how resonant X-ray scattering and diffraction enable to gain unique insight into the behavior of charge balancing counterions within mixed conducting systems. Indeed, with the first operando measurement at the Cl-edge (2.8 keV), we found that instead of counterion size, polymer charge state and associated ion and water interactions dictate counterion location. Specifically, ions reside far away from the electronic charge transporting polymer backbone at low doping and migrate to positions near the backbone with increased charging [4].

References

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- [2] G. Freychet, et al., Mater. Horiz. 9, 1649 (2022).
- [3] LQ. Flagg, et al., Chem. Mater. 35, 10, (2023).
- [4] D Meli, et al., Mater. Horiz. 9, 1649 (2025).