

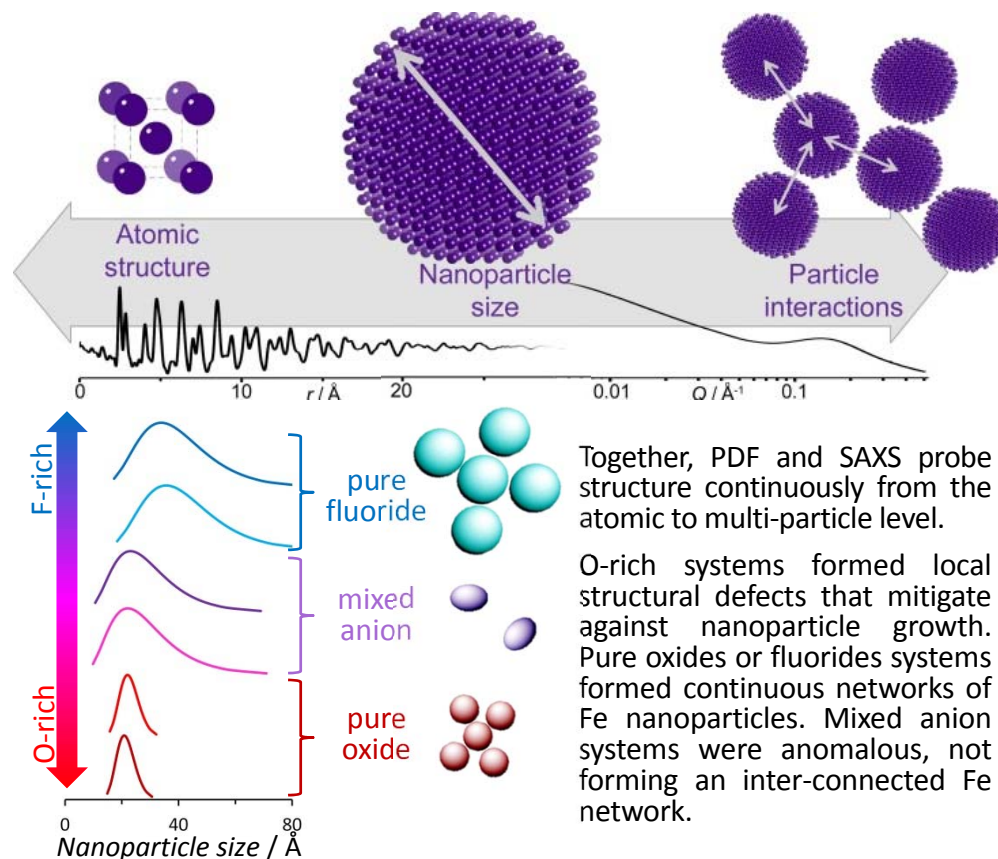
# Coupling of chemistry to atomic- and nanoscale structure in electrochemical conversion

## Scientific Achievement

By combining complementary hard X-ray tools, we resolve how anion chemistry (O vs F) influences the structure of metallic Fe<sup>0</sup>, formed in conversion electrodes, across multiple length-scales—from Ångstroms to tens of nm.

## Significance and Impact

Nanostructured metallic Fe both mediates electronic conductivity through the composite electrode and impacts battery cycle life. This work demonstrates how the anion chemistry of the initial electrode governs the Fe particle size and nanostructure by influencing defect formation, atomic mobility, particle annealing, and growth. These insights suggest a basis for the performance advantage of mixed-anion oxyfluorides and allow us to optimize both electronic conductivity and cycle life in next-generation battery electrodes.



## Research Details

Pure Fe oxides, Fe fluorides and mixed-anion Fe oxyfluorides were electrochemically lithated to form metallic Fe<sup>0</sup>. Pair distribution function (PDF) from 11-ID-B and small-angle X-ray scattering (SAXS) from 12-ID-B at Argonne's Advanced Photon Source were combined to probe structure of the resulting Fe<sup>0</sup> across multiple lengthscales.

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