Tracking Atomic-Scale Structural Evolution in Bimetallic Nanoparticles Using Deep Learning and X-ray Scattering

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Reconstructing nanoparticles (NPs) growth at the atomic scale in real time remains a long-standing challenge, especially for (multi)metallic systems that feature unconventional structures and complex spatial arrangements.[1]

In this talk, I will present a *methodology that integrates an X-ray scattering approach based on the Debye Scattering Equation (DSE)* [2,3] *with a deep learning (DL) regressor*, establishing a direct link between experimental data and data-driven structural interpretation. The developed approach enables the extraction of atomic-level descriptors, including size, composition, and elemental ordering of bimetallic NPs, using only X-ray scattering profiles as input. This makes the approach naturally suited for on-the-fly and high-throughput data acquisition.

Here, we apply this model to reconstruct the growth mechanism of Ag-Co NPs formed by Co vapor deposition onto Ag seeds, monitored *in-situ* by GIWAXS under out-of-equilibrium conditions. Our analysis reveals that the final NPs architecture is not determined only by the amount of Co supplied but instead *results from a kinetically governed evolution pathway.*

Overall, the developed framework removes the need for multiple complementary characterization techniques or iterative trial-and-error procedures, *enabling real-time, atomic-scale insights into nanoscale growth processes.*

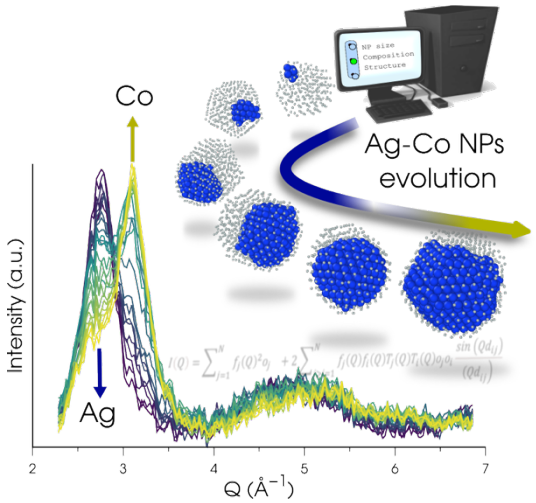


Figure 1. Predicted evolution of size, composition, and atomic-scale structure of bimetallic NPs based on the developed DSE–DL framework.

[1] R. Ferrando et al. *Chem. Rev.* 108 (2008) 845–910.
[2] F. Bertolotti et al. *Eur. J. Inorg. Chem.* 2018 (2018) 3786–3786.
[3] L. Allara, F. Bertolotti, A. Guagliardi, *Npj Comput Mater* 10 (2024) 54.