Structure of Atomically Precise Nanoclusters

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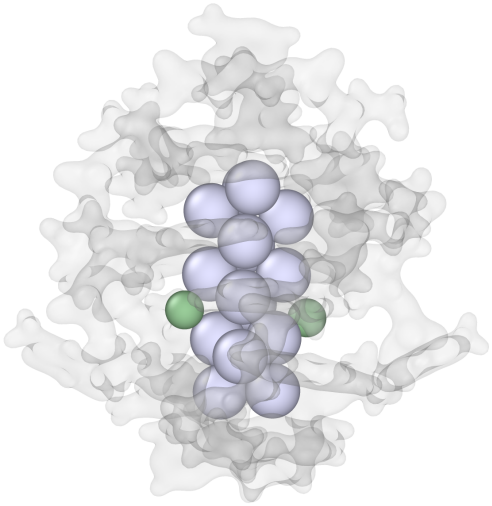
Nanoclusters occupy the unique size regime between molecules and bulk materials, exhibiting distinct structural and chemical properties. These clusters are often synthesized, manipulated, and applied in solution, where resolving their atomic structure presents a significant challenge. X-ray total scattering combined with pair distribution function (PDF) analysis offers a powerful route to overcoming these challenges, enabling atomic-level structural insights even for the smallest and most disordered systems. Despite its potential, routine structural determination of nanoclusters in solution remains an emerging capability.

In this contribution, I will highlight recent advances in structural analysis and data collection methods tailored for nanoclusters. These include the application of PDF techniques to DNA-stabilized silver nanoclusters[1] and metal-oxo clusters, as well as cutting-edge developments in ultrafast PDF measurements using X-ray free electron lasers[2]. I will also show how nanoclusters can serve as atomically precise building blocks for amorphous metal–organic frameworks (MOFs), enabling controlled incorporation of defects and structural disorder[3]. While focused on nanoclusters, the methodologies discussed have broad relevance for the structural study of other complex, disordered materials.



[1] A. F. Sapnik *et al.*, *Angew. Chem. Int. Ed.*, **2025**, e202422432.
[2] A. F. Sapnik *et al.*, *arXiv*, 2025. DOI: 10.48550/arXiv.2504.21462
[3] N. L. Baun *et al.*, *ChemRxiv*, 2025. DOI: 10.26434/chemrxiv-2025-psg4n