Single-Particle Diffraction with the X-Ray Free Electron Laser: New Opportunities to Study Structure and Function in Biology

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The X-Ray Free Electron Laser (XFEL) enables diffraction from individual biomolecules. The obvious advantage is that no crystals are required. But the true potential of single-particle diffraction unfolds in the presence of structural variability, intrinsic to biological function. Data analysis using manifold-based machine learning reveals the concerted structural changes and enables mapping the conformational spectrum, energy landscapes and compiling molecular movies. Performing single-particle diffraction in a time-resolved manner can further advance these salient opportunities.