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Creating and controlling cryogenically-cooled beams of shock-frozen, isolated, biological and artificial nanoparticles

Single-particle diffractive imaging (SPI) is emerging as a new technique for the three-dimensional (3D) imaging of aerosolized nanoparticles at x-ray free-electron lasers (XFELs). However, one of the primary bottlenecks in realizing SPI is the efficient delivery of isolated, reproducible target particles into the x-ray focus [1]. Here, we present novel approaches for the production of cold and high-density beams [2] of a broad variety of biological nanoparticles, ranging from single-domain proteins, including membrane proteins, to multi-subunit protein complexes and molecular machines, designed for use in XFEL experiments. This will also enable us to gain a better understanding of the ultrafast dynamics across extended biological systems. Fast freezing from ambient temperature to 10 K in less than 10 µs will help freezing room temperature equilibrium state distributions and even the trapping of reaction intermediates.

Furthermore, we have developed a numerical simulation infrastructure that allows the quantitative simulation of particle trajectories through the setup [3]. This allowed us to improve injection geometries and build aerosolinjection systems optimized for specific particle sizes in order to produce the highest-density particle beams [2, 4]. We propose an optimized setup with cooling rates for few-nanometers particles on nanoseconds timescales. The produced beams of shockfrozen isolated nanoparticles provide a breakthrough in sample delivery, e.g., for diffractive imaging and microscopy or low-temperature nanoscience. The produced cryogenically-cooled particle beams can subsequently be further manipulated and controlled using electric [5] or optical fields, such as hollow-core vortex laser beams [6].

[1] M. M. Seibert, *et al.*, *Nature* **470**, 78 (2011)
[2] A. K. Samanta, *et al.*, arXiv:1910.12606 [physics.bio-ph]
[3] N. Roth, *et al.*, *J. Aerosol Sci.* **124**, 17 (2018)
[4] V. Singh, *et al.*, *Phys. Rev. A* **97**, 032704 (2018)
[5] Y. P. Chang, *et al.*, *Int. Rev. Phys. Chem.* **34**, 557 (2015)
[6] N. Eckerskorn, *et al.*, *Phys. Rev. Appl.* **4**, 064001 (2015)

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