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Ultra fast atomic pair distribution function (PDF) analysis: a new chapter in the goal of atomic movies

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Abstract: It has long been a goal to obtain “atomic movies”, where frames are captured showing how atoms rearrange during after excitation. To do this, we need a camera that can “see” atoms, with a shutter speed and a frame-rate on the femtosecond time-scales, the time-scale of atomic motions. It has long been realized that diffraction is a way to see atoms, and XFELs allow us to do diffraction in a stroboscopic mode on femtosecond timescales. If you have a well defined crystal, you can use crystallographic methods to solve with high quantitative accuracy the average position of atoms in the crystal, and from the early dates of ultra fast x-ray studies there have been crysatllographic measurements that sought to follow atomic trajectories. However, if your target material is not a crystal but a molecule or a cluster of atoms or a nanoparticle, crystallography is no longer a good starting point for analyzing your diffraction data. The atomic pair distribution function (PDF) analysis of powder or single-crystal diffraction data is now highly developed for this purpose and has become widlely used in the chemical and materials science communities. The PDF function directly measures the relative positions of atoms in real-space and so, in principle, is a great option for making molecular movies. The measurements require wide ranges of diffraction/reciprocal space to measured with good precision using short-wavelength probe particles. All of these aspects present challenges for first generation XFELs. However, currently emerging are XFELs that can provide good flux of hard x-rays (˜30 keV energy for example) making in principle ufPDF a very real possibility. The short wavelength of electrons also suggests that ultrafast electron diffraction could be a explored for PDF analysis too. In this talk I will describe the PDF method and our intital attempts to measure and make corrections to data from LCLS to obtain quantitatively reliable PDFs on picosecond timescales. The experiment is to study the response of electronic dimers (a form of charge density wave) in a strongly correlated electron system, CuIr2S4. Initial results are very promising, suggesting that ufPDF could emerge as a highly promising, fully quantitative method for studying small clusters and molecules, opening the door to molecular movies of non-crystals

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