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Multiwavelength anomalous diffraction at high x-ray intensity

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The coherent x-ray scattering pattern of a molecule is connected to the modulus squared of the Fourier transform of the electron density of the molecule. The phase of this Fourier transform is not measured. As a consequence, a reconstruction of the electron density—and thus of the molecular structure—is not immediately possible. In x-ray crystallography at storage-ring-based synchrotron radiation sources, the multiwavelength anomalous diffraction (MAD) method is used to determine phase information by employing anomalous scattering from heavy atoms. X-ray free-electron lasers (FELs) provide the extremely high x-ray intensity required for revealing the structure of single molecules or nanocrystals, but the phase problem remains largely unsolved. A particular challenge is that, at high x-ray intensity, samples experience severe electronic radiation damage, especially to heavy atoms, which hinders direct implementation of MAD with x-ray FELs. In the first part of the talk, I will discuss how MAD phasing can be extended to high x-ray intensity [1]. The proposed technique relies on the existence of a Karle-Hendrickson-type equation in the high-intensity regime and requires the ability to computationally predict the x-ray-induced ionization dynamics of heavy atoms. In the second part of the talk, this ability will be put to the test. I will review x-ray FEL experiments that have been carried out on atomic xenon and will compare the observations to extensive first-principles calculations [2,3]. At sufficiently high photon energies, there is good agreement between experiment and theory. However, close to inner-shell edges, which play a key role for MAD phasing, specific discrepancies are found. A strategy will be discussed that is expected to allow us to eliminate these discrepancies.

[1] S.-K. Son, H. N. Chapman, and R. Santra, Phys. Rev. Lett. **107**, 218102 (2011).
[2] B. Rudek *et al.*, Nature Photonics **6**, 858 (2012).
[3] H. Fukuzawa *et al.*, submitted.