Multiwavelength anomalous diffraction at high x-ray intensity

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The determination of the atomically resolved 3D structure of proteins is a central goal of structural biology. X-ray crystallography has been widely used for structural determination, but it suffers from two bottlenecks: the phase problem and growing high-quality crystals. The multiwavelength anomalous diffraction (MAD) method with synchrotron radiation is used to determine phase information by employing resonant elastic x-ray scattering from heavy atoms. X-ray free-electron lasers (XFELs) show promise for revealing molecular structure without the need for large-scale crystals, using femtosecond x-ray nanocrystallography [1], but the associated phase problem remains largely unsolved. Because of the extremely high intensity of XFELs, samples experience severe and unavoidable electronic radiation damage, especially to heavy atoms, which hinders direct implementation of MAD with XFELs.

I will discuss how the MAD phasing method can be extended to the high x-ray intensity [2]. The proposed method requires the ability to describe the dynamical behaviour of heavy atoms in high-intensity hard-x-ray beams [3,4]. The XATOM toolkit [5] is used to simulate detailed electronic damage dynamics of heavy atoms (Fig. 1). In this talk, I will demonstrate the existence, in spite of the high degree of ionization, of a key equation for MAD in the high-intensity regime. I will present brand-new phasing methods, because of the high degree of ionization, are achievable in femtosecond x-ray nanocrystallography with XFELs.

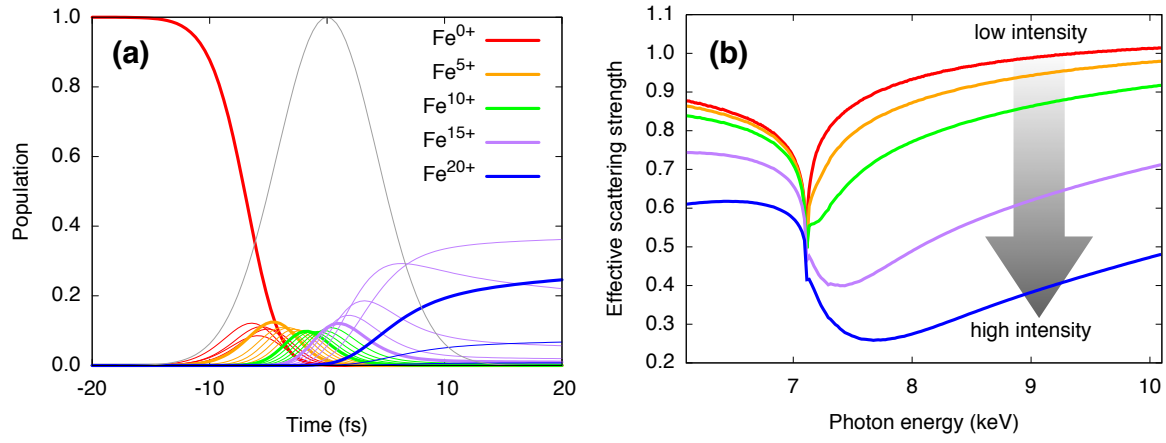

Figure 1: (a) Population dynamics of Fe charge states during an ultrashort high-intensity x-ray pulse. (b) Dramatic changes in effective scattering strength of Fe as the intensity increases.

References

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