White Paper
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A Dedicated Soft X-ray Beamline at APS for Native SAD Phasing and Multi-Dimensional Crystallography Combing X-ray Diffraction and X-ray Absorption Spectroscopy

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1. **Abstract**

The scientific need for a dedicated soft X-ray beamline at the APS for Native-SAD phasing of macromolecules was the focus of our Letter-of-Intent in 2010. Through discussions and proof-of-concept studies another uncharted area of scientific exploration, equivalent to site-specific X-ray absorption spectroscopy, is now possible. This is achieved by collecting a number of diffraction data sets at wavelengths that span a metal's X-ray absorption edge and analyzing the metal's anomalous scattering signal. The 4D (position and spectral) information for many elements that are important to biological systems can be obtained using X-rays in the range from 1.48 to 3.10Å. Our proposed upgrade is conceptually equivalent to upgrading from a visible-light black-and-white camera to a color camera (position & spectrum) and offers significant opportunities for advancing new science in biology, chemistry, physics and engineering via its added capability of recording the electronic spectrum of metal atoms by diffraction.

2. **Science Case**

I. Native SAD Phasing is Maturing

Native single-wavelength anomalous diffraction (Native-SAD) phasing uses the anomalous scattering signal of atoms in the native crystalline samples of macromolecules, recorded from single-wavelength X-ray diffraction experiments. These atoms include sulfur and other light atoms found in native protein,