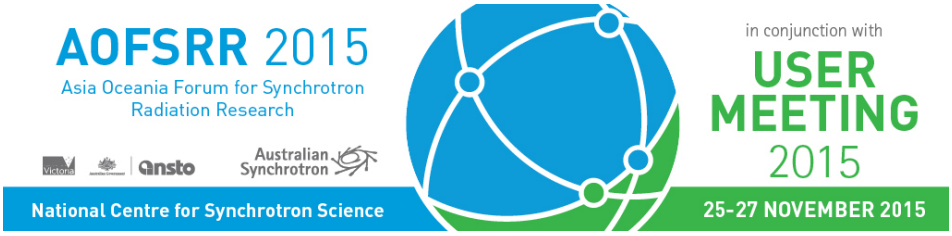


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# FDMX: Full-Potential Calculations of EXAFS for Extraction of Structural, Thermal, and Electronic Properties from Absolute Accuracy Measurements

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We present the new computational package FDMX; a full-potential code for accurate robust calculations of x-ray absorption fine structure across all energies from below the edge to the smooth atom-like absorption region.
Full-potential modeling of condensed matter systems is a critical tool for analysis of x-ray absorption near-edge structure (XANES) spectra [1,2]. Despite demonstrated advantages in the low-energy regime [3], these tools are still not generally applied to EXAFS analysis.
We present here the new package FDMX, a development of the Finite Difference Method for Near-Edge Structure (FDMNES) package [2], for use in the calculation of extended XAFS spectra. FDMX features new implementations of thermal and electron scattering parameters [4], core-hole and outer-shell absorption effects. FDMX calculates high-accuracy XAFS spectra for large energy ranges in both elemental and complex molecular systems. Material parameters such as bond lengths, electron inelastic mean free paths [5], and Debye-Waller factors [6] may be extracted using full-potential modeling.
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## Keywords

FDMX FDMNES XAS full-potential thermal parameters

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