

## **CLS-SGM Phosphorus K-edge X-ray absorption near-edge spectroscopy (XANES) and valence band photoemission spectroscopy (PES) of intermetallic compounds**

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The electronic structure of many transition-metal phosphides and arsenides is difficult to examine because of their metallic character and significant polar covalent character in their bonding. Through XANES and PES, valuable information has been obtained on several binary and ternary compounds of the form MP,  $M_{1-x}M'_xP$ , and  $MA_{1-y}P_y$  (M, M'=Ti – Co, with M being more electronegative than M') and on the new compound  $HfSi_{0.5}As_{1.5}$ . In the MP series, P K-edge XANES conducted on the SGM beamline showed that the P K-edge energy decreases linearly through the sequence from CoP to TiP. This occurs because the ionic character of the M-P bond increases as the metal is changed from Co to Ti, allowing for greater screening of the P nucleus. The P K-edge energies in the pseudobinary series,  $M_{1-x}M'_xP$  and  $MA_{1-y}P_y$ , are lower than in the binary analogues. This deviation arises from the contribution of next nearest neighbour (second coordination shell) atoms to the potential experienced by the P atoms, which is modified because of charge transfer between the two dissimilar metals and variation in the ionic character of M-Pn (Pn=P, As) bonds.

PES conducted on the SGM beamline also provided valuable insight into the charges of constituent atoms in  $HfSi_{0.5}As_{1.5}$ , through examination of the change in peak intensities in the valence band spectrum as the cross-section is varied with different excitation energies (500 – 250 eV). Analysis of these spectra revealed that the Hf 5d band is partially occupied. This result argues against the fully ionic formulation  $[Hf^{4+}(Si_{0.5}As_{0.5})^1-As^{3-}]$  in which Hf relinquishes all of its valence electrons to the anions and instead supports the formulation  $[Hf^{2+}(Si_{0.5}As_{1.5})^2-]$ .

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