## LETTER

## Minimum XPS core-level line widths of insulators, including silicate minerals H.W. NESBITT,<sup>1,\*</sup> G.M. BANCROFT,<sup>2</sup> R. DAVIDSON,<sup>3</sup> N.S. MCINTYRE,<sup>2,3</sup> AND A.R. PRATT<sup>4</sup>

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## ABSTRACT

A monochromatic AlK $\alpha$  source and magnetic confinement charge compensation yield an As 3d line width of 0.52 eV for the bulk insulator As<sub>2</sub>S<sub>3</sub> (orpiment) which is as narrow as the As 3d line width obtained for the semiconductor FeAsS (arsenopyrite). These results, and the XPS results for silicates, demonstrate that charge broadening of XPS spectra has been overcome for most insulators provided care is taken with sample preparation. XPS core level spectral investigations of these minerals now may be conducted at the same level of detail as have been conducted on semi-conductors and metals.

The Si 2*p* spectrum of a non-conducting orthosilicate (Mg-rich olivine) displays a total line width of 1.36 eV compared to very high resolution synchrotron XPS line widths of 1.1 eV for an Si 2*p* spectrum of gaseous Si(OCH<sub>3</sub>)<sub>4</sub>, and 1.42 eV for the Si 2*p* peak of non-charging SiO<sub>2</sub> thin-films grown on Si metal. These results demonstrate that Si 2*p* peak broadening of these silicates does not result from differential charging. Comparison of the Si 2*p* spectrum of Si in olivine which contains non-polymerized, independent SiO<sub>4</sub> tetrahedra, with that of a gaseous analogue, Si(OCH<sub>3</sub>)<sub>4</sub>, also composed of non-polymerized Si atoms tetrahedrally bonded to O, provides insight into the cause of Si 2*p* peak broadening for olivine (and probably for all other silicates). The vibrational contributions to the Si 2*p* spectrum of Si (OCH<sub>3</sub>)<sub>4</sub> were used to fit the Si 2*p* peak of olivine, with each vibrational contribution broadened to reflect the minimum line width of the XPS instrument. Although the Si 2*p* envelope resulting from this procedure yields a reasonable fit to the olivine Si 2*p* spectrum of olivine. Continued development of the technique should allow determination of transition metal oxidation states and other chemical state properties of non-conductor Al-silicates.