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| PI Name | Elizabeth Gibson |
| PI Number | 010-21 |
| Application Number | 20210429-010-21 |
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| Application Title | |
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| Experiment description |
| XPS data collection was performed at the EPSRC National Facility for XPS (‘HarwellXPS’), operated by Cardiff University and UCL, under contract No. PR16195. |

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| Results |
| Provided as Casa files |

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| References |
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| Instrument Settings | |
| Instrument make/model | Kratos Axis Supra |
| X-ray source | Mono Al kα |
| X-ray source energy | 1486.7 eV |
| X-ray source strength | 180 W |
| X-ray source spot size | 700 µm x 300 µm |
| Analysis spot size | 700 µm x 300 µm |
| Charge control | Electronic charge neutralization using low energy flood gun and magnetic immersion lens. Filament current = 0.38 A, charge balance = 2 V, filament bias = 4.2 V. |
| Analysis pressure | 9 x 10-9 Torr |
| Analyser type | Spherical sector |
| Detector | Multichannel resistive plate |
| Number of detector elements | 3 MCP, 128 channel DLD |
| Temperature during analysis | 294 K |
| Survey spectra pass energy | 160 |
| Region spectra pass energy | 20 |
| Mounting/ex-situ preparation | Samples affixed to copper tape |
| In-situ preparation | N/A |
| Elements analysed | C, O, Re, Ru, Pt, Ni, Ir |
| Auger regions analysed | N/A |
| Samples analysed | 14 |

**Experimental**

XPS data was acquired using a Kratos Axis SUPRA using monochromated Al kα (1486.69 eV) X-rays at 15 mA emission and 12 kV HT (180W) and a spot size/analysis area of 700 x 300 µm. The instrument was calibrated to gold metal Au 4f (83.95 eV) and dispersion adjusted give a BE of 932.6 eV for the Cu 2p3/2 line of metallic copper. Ag 3d5/2 line FWHM at 10 eV pass energy was 0.544 eV. Source resolution for monochromatic Al Kα X-rays is ~0.3 eV. The instrumental resolution was determined to be 0.29 eV at 10 eV pass energy using the Fermi edge of the valence band for metallic silver. Resolution with charge compensation system on <1.33 eV FWHM on PTFE. High resolution spectra were obtained using a pass energy of 20 eV, step size of 0.1 eV and sweep time of 60s, resulting in a line width of 0.696 eV for Au 4f7/2. Survey spectra were obtained using a pass energy of 160 eV. Charge neutralisation was achieved using an electron flood gun with filament current = 0.38 A, charge balance = 2 V, filament bias = 4.2 V. Successful neutralisation was adjudged by analysing the C 1s region wherein a sharp peak with no lower BE structure was obtained. Spectra have been charge corrected to the main line of the carbon 1s spectrum (adventitious carbon) set to 284.8 eV. All data was recorded at a base pressure of below 9 x 10-9 Torr and a room temperature of 294 K. Data was analysed using CasaXPS v2.3.19PR1.0. Peaks were fit with a Shirley background prior to component analysis.

**Acknowledgments**

The X-ray photoelectron (XPS) data collection was performed at the EPSRC National Facility for XPS (“HarwellXPS”), operated by Cardiff University and UCL, under Contract No. PR16195.