Durham X-ray Absorption Facility (DXAF) – Newsletter April 2023



Welcome to the April instalment of the DXAF newsletter. The facility has been growing on all angles, with the introduction of new users, new software updates and the development of new cells! The newsletter will now become a bimonthly event so it will be jam packed with information which may interest you!

What has been going on?

Progress update on our first *in situ*!

We are working on the development of a cell capable of *in situ* characterisation (gases / temperature). This cell is currently in the design phase and is envisioned to be capable of taking a pellet-based sample up to temperatures of at least 400 °C (based on cartridge heaters rated to 500 °C) under various gas feeds. The facility will keep you posted about the development of this cell and when it will be available for users, but in the meantime we are very happy to discuss possible samples!

DXAF on tour

DXAF was happy to engage with the EXAFS community at the latest Collaborative Network for X-ray Spectroscopy (CONEXS) event in Oxford, UK. This EPSRC funded network aims to bring together experimentalists and theoreticians working within the X-ray spectroscopic community to achieve new levels of understanding, especially for the interpretation of experimental data and the use of high-powered computing (HPC). Please check them out if you don't already know about them.



Growing user base!

The growth of new users has been great for the facility. Thank you all so much for spreading the word about the facility! We have currently got users spanning across the UK, from Glasgow to Oxford. If you feel like you or your colleagues may benefit from using the facility, please get in touch!



Fig. 2: Growing map of the DXAF's UK userbase.

What is coming up?

DXAF has recently upgraded the software using for data acquisition and analysis. The new easyXAFS software, has the following updated features:

- 1) new integrated hard X-ray control with better functionality;
- 2) advanced alignment procedure for sub-mm positional stability;
- 3) sample pellet homogeneity tester;
- 4) cropping data and background subtraction.

Our facility can't wait to try the new features to see how it will benefit how we analysis your data and how data processing can be improved!

Conquering the periodic table one spectra at a time

We have seen many users provide sample to the facility based on early row transition metal species. The facility is keen to understand how the easyXAFS can handle other elements, so could your sample fit this role? Please get in contact

1 H Hydrogen										² He							
³ Li Lithium	4 Be Beryllium				i .	_0	Р		2			5 B Boron	Carbon	7 N Nitrogen	8 Oxygen	9 F Fluorine	Ne Neon
¹¹ Na ^{Sodium}	12 Mg Magnesium					-C		9	5			13 Aluminium	¹⁴ Si silicon	¹⁵ P Phosphorus	16 Sulfur	17CI Chlorine	18 Ar Argon
19 K Potassium	Ca Calcium	21 Sc Scandium	22 Ti Titanium	23 V Vanadium	24 Cr Chromium	25 Mn Manganese	Fe tron	27 Co Cobalt	28 Ni Nickel	29 Cu Coppe	30 Zn Zinc	³¹ Ga _{Gallium}	³² Ge	Arsenic	34 Se Selenium	35 Br Bromine	36 Kr Krypton
37 Rb Rubidium	38 Sr Strontium	39 Yttrium	40 Zr Zirconium	41 Nb Niobium	42 Mo Molyb- denum	43 TC Technetium	44 Ru Ruthenium	45 RH Rhodium	46 Pd Paladium	47 Ag silver	48 Cd Cadmiu	m 49 Indium	Sn Tin	S1 Sb Antimony	52 Te Tellurium	53 I Iodine	54 Xe Xenon
55 Cs Cesium	56 Ba Barium	57-71 *	72 Hf Hafnium	73 Ta Tantalum	74 W Tungsten	75 Re Rhenium	76 Os Osmium	77 Ir Iridium	78 Pt Platium	79 Au _{Gold}	80 Mercur	y 81 Thallium	82 Pb	83 Bi Bismuth	84 Po Polonium	85 At Astatine	86 Rn Radon
87 Fr Francium	88 Ra Radium	89-103 **	104 Rf Ruther- fordium	105 Db	106 Sg Seaborgium	107 Bh ^{Bohrium}	108 Hassium	109 Mt Meitnerium	110 Ds Darmst- adtium	111 Roent geniur	112 Copernic	n um Nihonium	114 Flerovium	115 Mc Moscovium	116 LV Livermorium	117 TS Tennessine	118 Oganesson
57 58 59 60 61 62 63 64 65 66 67 68 69 70 71																	
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Fig. 3: Potential sample edges DXAF can conduct XAFS analysis for.

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Useful links:

https://www.easyxafs.com/ https://research.ncl.ac.uk/conexs/about/ Durham Uni DXAF website coming soon