Preliminary course plan for

**LINXS XAS school**

Winter School on

Practical EXAFS and XANES,

Hands on training in Design, Performance and Analysis and of XAS experiments

Monday Nov 1st – Friday Nov 5th 2021

| DAY1 | |
|---|---|
| Introduction to course | |
| Introduction to x-ray based techniques | What are X-rays and why do we bother |
| | General interaction of X-rays with Matter (scatter, absorb, ionize (photon and electron emission) for different elements and at different energies consider time scales |
| | Characteristic vs general absorption (imaging), introducing edges |
| | Soft vs hard vs electrons (general) (information depth and type) |
| | Information from XPS |
| | Information from XRF |
| | Information from XDS (crystal and diffuse) |
| | Information from XAS and XES (lecture in a slide) and examples |
| Sources of X-rays | Characteristic vs broad band radiation |
| | X-ray tubes |
| | Accellerate and trap electrons |
| | Bending magnets, field dependence, directionality |
| | Wiggler |
| | Undulator |
| | XFEL |
| | Compare numbers and type of radiation |
| Detection of x-rays | Reprise Interaction |
| | Amplification curve (recombination, extraction, amplification, breakthrough) |
| | GM-counter/SDD as counter |
| | Linear devices (diodes) Ionization chambers |
| | energy proportional detectors SDD / CCD limitations, strength |
| | Bragg and Laue (coarse) for monochromator, mention higher harmonics |
| | Flat and bend crystals. For analysis |
| | Geometry considerations (resolution vs efficiency) |
| | Comparison of detection techniques, which for what task, combination? |
| | Optics surface (reflectivity) |
| | Optics KB/toroid/Zone plate |
| | Optics Microcapillary |
| XAS intro, XANES vs EXAFS | Reprise Interaction |
| | Reprise Information |
| | Beer lambert |
| | Types of XAS (transmission, vs Fluoresence, vs Electron) |
| | Mention Self-absorption in fluorescence-detected XAS spectra |
| | Scientific questions, scientific samples, sample types. |
| XAS at BALDER | Sources, optics, mono (choices) optics |
| | How/where to read beamline informations |
| | detectors, with link how does this look at Balder |
| | sample environments |
| Sample consideration | Sample x-ray thickness |
| | environment absorption |
| | Intro to calculation tool (hephaetus or similar) |
| | optimal/real conditions |
| | practical preparation solid (Balder focus) |
| | practical preparation liquid/gas choices (Balder focus) |
| | sample damage |

| DAY2 | |
|---|---|
| EXAFS introduction | Reprise Interactions |
| | Fermis Golden Rule in one electron transitions, |
| | Allowed and forbidden transitions, use applet to visualize, white line, mention quadrupol, mention polarization |
| | XANES examples (edge shift, pre-edge peaks, white line) |
| | EXAFS equation walkthrough |
| | Frequencies and Phases (link to Feff and elements, mention non-spherical) |
| | Signal decay (DW and longer path), discuss K-weights |
| Data-reduction with Athena | What is Athena used for, what software is available |
| | Opening Data - text files, transmission, fluorescence |
| | Inspecting data for artifacts, deglitching |
| Principles and procedures | E0 with example foil |
| | Pre-edge, post-edge, norm |
| | Extraction |
| | Fourier transform: |
| | Principle based on EXAFS equation. |
| | Complex numbers, magnitude and phase |
| | Windows, k-range, k-weights, filtering |
| FEFF input file For EXAFS | EXAFS fits based on path expansion |
| | Molecule/crystal structure files |
| | Atoms |
| | EXAFS cards and output |
| | Path generation in Artemis |
| | Path plotting and selection |
| | Single shell fitting |
| **Practical Athena Artemis first time** | **Get to Fourier transform (follow tutorial) - Ferrocene** |
| | **Get to Fourier transform (follow tutorial) - Ferrocene with glitches** |
| | **Get to Fourier transform (follow tutorial) - Ferrocene with shift** |
| | **Artemis first shell fit Get one parameter (follow tutorial) - Ferrocene** |
| | **Artemis multiple paths (follow tutorial) - Ferrocene** |
| Discussion | |
| **Practical Athena Artemis Atoms** | **simple crystal data Atoms FEFF** |
| | **Fit simple Crystal** |
| | **Fit second Crystal with Glitches and shift** |
| Discussion | summary of what was done, pitfalls |

| DAY3 | |
|---|---|
| Questions from homework | |
| LCA | Introduction linear combination Analysis XRF/XANES/EXAFS |
| PCA | Show PCA and machine learning |
| **Analyzing mixed material Data** | **Tutorial Linear combination XRF** |
| | **LCA XANES/EXAFS** |
| Discussion | |
| Planning a beamtime/proposal | Defining a Question |
| | How long do things take? |
| | Achievable S/N for (a) transmission and FY detection, (b) XANES and EXAFS and (c) concentrated and diluted samples. |
| | What reference Samples do I need |
| | What numbers do I need |
| | What resources do I need |
| | Where do I find information |
| Quality of Fits, what are parameters | Information theory about fit quality, and judging what is good. |
| | Approach to measurements: what quality is sufficient? |
| Publishing/reporting data | Databases, standard plots, crystallogrpahic files |
| Beyond the simple a look over the rim. | Muffin tin and the expansion with greens function, non spherical potentials |
| | Full multiple scattering calculations and their tools (GNXAS?) |
| | What are parameters, how can we judge when we have to many |
| | |
| **Preparation of experiments** | **Calculate the numbers for a proposal for the experiment** |
| | **Calculate determine the experimental parameters for the experiment** |

| DAY4 - MAX IV - Practical Day | |
|---|---|
| **A-SET MAXIV** | **B-SET LINXS** |
| **Practical sample prep grinding** | Multiple scattering/ focusing effect: cubic pervoskite and play with angle |
| **Practical sample prep mounting** | Multiple edges in one spectrum (Cu/Zn, Mn/Fe) |
| break | Self Absorption and correction: hematite XANES and EXAFS, fitting coordination number |
| **Beamline Instructions, Safety instructions** | Lunch and move and MAXIV Tour |
| **Measurement** | |
| **A-SET LINXS** | **B-SET MAXIV** |
| Lunch and move and MAXIV Tour | **Practical sample prep grinding** |
| | **Practical sample prep mounting** |
| **Working serious problem Molecules (many data-sets)** | break |
| | **Beamline Instructions, Safety instructions** |
| | **Measurement** |

| DAY5 | |
|---|---|
| **DataAnalysis training** | LCF: three different examples from ashes, in situ, CZTS |
| Discussion | |
| **Data Analysis big project** | Particle size vs coordination number, Pd (foil to NP), Lindsays science example |
| Discussion | |
| Teacher Presentation of Exam problems | **data from practical experiment at Balder** |
| End of Course | |

| DAY6 (half day) examination | Presentation of study project in smaller groups |
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