| **O-02** | **Mon. 16. 06., 12⁵⁰-13¹⁰** |

O-02   **Mon. 16. 06., 12^{50}-13^{10}**

X-ray absorption fine structure study on electrochromic metallo-supramolecular polyelectrolytes

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Keywords: XAFS, electrochromism, structure, spin crossover, charge transfer

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Rigid rod type metallo-supramolecular coordination polyelectrolytes with divalent $3d$ metal centers (MEPE) exhibit remarkable electrochromic properties. The Fe-MEPE changes its color from blue to transparent, when an electric potential is applied to the material. In the case of Co-MEPE the change is from red to transparent. These materials are prospective candidates for application in so called smart windows that can be shaded on demand for e.g. privacy protection, large scale displays, and energy conservation in vehicles and buildings.

A comprehensive x-ray absorption fine structure (XAFS) study was made *in situ* and *in operando* on annealed MEPE powders and working electrochromic devices, respectively. It has been found that during annealing at temperatures above 100 °C a rearrangement of the ligands around the metallic center occurs without a redox reaction, but due to spin crossover only. The atomic positions and the alignment of the ligands with respect to the metallic center in the two states have been determined by use of first principle calculations.

The *in operando* experiments revealed that during the switching process from blue to transparent the metallic center changes its formal valence from 2+ to 3+. The charge transfer is not accompanied by any change in the local structure.
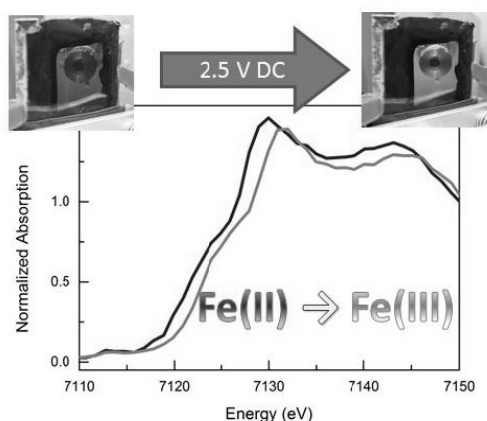

Figure 1. XANES of the *in operando* experiment on Fe-MEPE.

O-03   **Mon. 16. 06., 11^{30}-11^{50}**

Eu-XFEL upgrade

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Keywords: FEL, Tesla, cavity, beam dynamics

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The talk presents beam properties calculation for the superconducting linear particle accelerator of free electron laser POLFEL [5] and possible XFEL [8] upgrade. Normalized slice emittance and bunch size are tracked for the 1.6-cell superconducting injector with solenoid followed by 2-structure cryomodules[3] of HZDR-type.

Main results are taken from ASTRA [2] 2D calculations. First the cavity and solenoid were tested in order to find the most suitable parameters. The criterion for optimization was normalized slice emittance. The key parameter is an inclination angle of the cavity rear wall to the longitudinal axis. During performed studies the 8 degree inclination angle was chosen as an optimal value for further test. Next the cryomodules were added and the beam size was honed due to its great focusing and reaching values near zero. We targeted the beam size instead of emittance, since computation results, after adding cryomodules, show almost no influence on emittance.
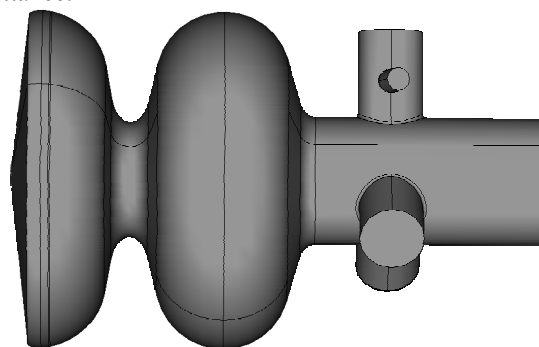

Figure 1. Tesla - type 1.6 cell cavity of electron gun.

Based on cavities shapes taken from FEM[6] program we made the 3D model of the accelerating structure using Microwave Studio [4] software. We tuned the model to match the calculations performed by Sekutowicz [7]. Then added the couplers. We do also have a model of Tesla - type 1.6 cell cavity of electron gun (Fig 1.). It was made using Cubit software [1] and exported to Microwave Studio. The goal is to build the same model as in ASTRA and to compare the emittance from both 2D and 3D modelling.

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