

## CH-6525- Photoresponsive Fe-Organic MOF materials

During the experimental time, we have done the ex-situ 1s2p RIXS measurements at the iron pre-edge region of various metal-organic thin-film samples as proposed. The samples that we measured were thin films deposited through atomic-molecular layer deposition technique. The samples included photoactive crystalline iron-azobenzene (Fe-AZO) or iron-stilbene (Fe-Stilb) films of a previously unknown metal-organic framework (MOF) type crystal structure. In addition to these photoactive MOF's, we have also studied another interesting iron-terephthalate (Fe-TP) MOF material. In total, we had 18 samples and two of the photoactive samples were measured before and after UV-irradiation. The as deposited trans isomer of both iron-azobenzene and iron-stilbene was irradiated for 1.5 h after the first measurement and the obtained cis isomer then subjected to RIXS measurement. So, in total we did 20 measurements, utilizing all the allocated shifts (15 shifts). There were no technical issues throughout our measurements, and we were able to proceed the experiments as we have planned.

For iron-azobenzene (Fe-AZO) MOF thin films, we had six samples deposited at three different temperatures (260, 280 and 300 °) and with different cycles of deposition (20 or 150). The thickness of the films measured was either  $\approx 50$  or  $\approx 350$  nm. We wanted to check how the deposition temperatures affects the coordination of iron and the ratio of  $\text{Fe}^{3+}/\text{Fe}^{2+}$  in these samples. The sample with 20 cycles deposited at 280 ° was used for trans-cis isomerization studies.

In case of iron-stilbene (Fe-Stilb) MOF films, we measured six samples deposited at two different temperatures (260 and 280 °). The samples were of different thickness ranging between 30-120 nm. The sample with 30 nm thickness deposited at 260 ° was used for trans-cis isomerization studies.

In case of iron-terephthalate (Fe-TP) MOF films, we measured six samples deposited at three different temperatures (250, 280 and 300 °) and with different cycles of deposition (50 or 300). The thickness of the films measured was either  $\approx 50$  or  $\approx 300$  nm. Since the crystallinity of these samples varied with deposition temperature, we were interested in finding out how the coordination of iron and the ratio of  $\text{Fe}^{3+}/\text{Fe}^{2+}$  in these samples are also changing with crystallinity. The results from iron-terephthalate samples are very soon going to published as the manuscript is currently in progress.

Overall, we have effectively utilized the allocated experiment time.