[MS24-P24] An in-situ study of host-guest interactions using a laboratory X-ray diffraction system

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Materials that are capable of facile hydrogen uptake and release promise safer alternatives for the concentration, storage and handling of hydrogen gas than those currently in everyday use. The design of novel materials for this purpose relies on understanding the host-guest interactions. Investigating structural modification under gas pressure by X-ray diffraction (XRD) is a technique that is ideally suited to study such interactions, particularly where it is possible to undertake such studies on a bulk powder sample rather than in the single crystal paradigm. The phase transitions recorded during the in situ measurements are instrumental to understanding the sorption-processes and reaction mechanisms. Furthermore, rapid X-ray diffraction data collection allows the determination of intermediate phases, onset points of reactions and information about the reversibility of sorption processes.

To date in situ high-pressure XRD studies are mainly performed at synchrotron facilities or are limited to the single-crystal environment[1]. In the work reported here we present structural transformations that were studied under high pressures of H2 using a standard laboratory X-ray diffraction system equipped with: (i) a sample chamber for X-ray diffractometers allowing gas pressures up to 100 bar and temperatures as high as 900 °C; (ii) hard radiation on a laboratory system, in this case molybdenum radiation and (iii) multi-dimensional X-ray detectors for rapid data collection.

1. see for example Jacobs, T. et al. Angew. Chemie. Int. Ed. (2012) 51, 4913 – 4916.