

Fysikermøtet 2023

Abstracts for Condensed Matter and Atomic Physics



Friday (Room: D) **OBS! 25 min talks+5min questions**

10:00 Abhishek Banerjee (University of Stavanger (UiS)): Deciphering Atomic Structure and Hydrogen Sorption Kinetics and Uptake of TiFe-Nb doped Metal-Alloys utilizing Combined Techniques: Synchrotron PXRD, EXAFS and First-Principle DFT calculations.

Hydrogen storage remains a challenge in the hydrogen economy due to its light weight and density. Metal alloys, particularly titanium-iron (TiFe), have emerged as a viable option for hydrogen storage at ambient conditions. TiFe is known for its ability to reversibly store hydrogen at room temperatures, with comparable volumetric capacities as that of liquid H₂. However, its relatively low gravimetric capacity and oxide formation present drawbacks for TiFe as a standalone storage material. To overcome these challenges, researchers have proposed elemental doping and post-mechanical processing. Theoretical studies have suggested that incorporating transition elements such as V and Nb as dopants in TiFe can enhance its hydrogen storage properties. By replacing Fe and Ti in the lattice, these dopants increase lattice size and strain, creating favourable diffusion pathways for hydrogen. However, there is limited research on TiFe doped with element Nb, and a comprehensive understanding of the correlation between its crystallographic structure and hydrogen storage properties is still lacking.

In this study, TiFe samples with varying Nb stoichiometries were synthesized using vacuum arc-melting (VAM). Characterization techniques including powder X-ray diffraction (XRD) and Extended X-Ray Absorption Fine Structures (EXAFS) analysis were employed. First principle Density Functional Theory (DFT) calculations using projected augmented wave (PAW) were performed to determine the location of Nb in the crystallographic structure of TiFe before and after hydrogenation. The results demonstrated showed high correlation between structural refinement achieved through PXRD and EXAFS analysis. H₂ absorption measurements conducted at temperatures and pressures of 55 °C and 40 bars respectively, showed that precise doping of TiFe with Nb significantly improved activation and kinetics without compromising its overall hydrogen sorption capacities. These findings contribute to a better understanding of Nb occupancy in the crystallographic structure of TiFe and its impact on hydrogen storage.

10:30 Diana Lucia (University of Stavanger): 1D Magnetism in Pauflerite

Pauflerite, or β -VOSO₄ was discovered among volcanic products of the Tolbachik volcano in Kamchatka [S. V. Krivovichev, et al., *Canad. Mineral* 2007, 45, 921]. It crystallizes in the Pnma orthorhombic group and its structure represent three dimensional frameworks built up from distorted V₄+O₆ octahedra and SO₄ tetrahedra. The V₄+O₆ octahedra share the O(2) corners to form [V₄+O₅] chains extending along the a-axis [Paufler, et al., *Z. Kristallogr.* 2014; 229(11): 725–729].

Diffuse scattering indicates that such defects are correlated and form thin layers, destroying alternation of V-O bonding pattern in the neighbouring chains. Using direct Monte Carlo (MC) modelling, we present here an atomistic realization of the disordered crystal structure [*Acta Cryst.* (2022). B78, 842-847].

The vanadium arrangements form low dimensional ladders with a nearest neighbor distance of 3.7Å and next near neighbor distance of 4.89Å (see Fig. 1). We have grown mm-sized single crystals of in β -VOSO₄ by following the method described by Peter Paufler, et al., [*Z. Kristallogr.* 2014; 229(11): 725–729]. V₄⁺ ions have spin ½, and present a well-defined orbital ground state, a spin only magnetism and weak spin-orbit coupling. Magnetic susceptibility and high field magnetization are in perfect agreement with theoretical expressions for 1D s-1/2 Heisenberg chain with an exchange parameter of 3.85meV and saturation fields over 60T. Powder inelastic neutron scattering shows clear gapless spinons with a continuum spanning up to 12meV. Thus, showing that Pauflerite is a realization of an ideal 1D s-1/2 Heisenberg chain.

11:00 Sofiia Bercha (Department of Mathematics and Physics, University of Stavanger): Combining in situ Raman and EXAFS studies: case of Ce-Zr Fumarate formation in water

Zr-based MOFs have gained recognition for their superior stability and rigidity, particularly in severe operating conditions, whereas their Ce-based counterparts possess exceptional redox activity but are generally less stable. Combining these two desirable attributes through the synthesis of a bimetallic Ce-Zr MOF holds great promise for the vast types of applications. Yet such a task has proven to be difficult since synthesis conditions for the two analogues differ drastically (Lammert et al., 2017; Nouar et al., 2015) .

In this work we have combined the in situ Raman and EXAFS studies to shed light onto the stages and formation mechanism of mixed Ce-Zr fumarates when using green water-based synthesis. Our findings show that Raman spectroscopy can be an excellent tool for the following of the MOF synthesis in industrial applications. EXAFS technique is element specific and allows to determine the stoichiometry of the mixed-metal MOF cornerstones (Lomachenko et al., 2018). When applied in situ, it can follow all the stages of the MOF formation in real time. Combination of these powerful techniques and additional characterisation with powder diffraction, electron microscopy, thermogravimetry and N₂ sorption at 77 K allow us to paint a full picture of the formation of Ce-Zr fumarates in water.

Lammert, M., Glißmann, C. & Stock, N. Tuning the stability of bimetallic Ce(IV)/Zr(IV)-based MOFs with UiO-66 and MOF-808 structures. *Dalton Transactions* 46, 2425–2429 (2017).

Nouar, F. et al. Tuning the properties of the UiO-66 metal organic framework by Ce substitution. *Chemical Communications* 51, 14458–14461 (2015).

Lomachenko, K. A. et al. Exact Stoichiometry of Ce x Zr 6-x Cornerstones in Mixed-Metal UiO-66 Metal–Organic Frameworks Revealed by Extended X-ray Absorption Fine Structure Spectroscopy. (2018) doi:10.1021/jacs.8b10343.