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**VABILO NA PREDAVANJE
V OKVIRU DOKTORSKEGA ŠTUDIJA
KEMIJSKE ZNANOSTI**

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z naslovom:

Solid-state hydrogen storage

v sredo, 25. januarja 2017 ob 15:00 uri
v predavalnici 1 v 1. nadstropju Fakultete
za kemijo in kemijsko tehnologijo, Večna pot 113

Vljudno vabljeni!

Abstract:

Hydrogen economy or hydrogen society is a combination of production, storage, delivery and use of hydrogen as an energy carrier. Hydrogen can be used to store and transport an excess energy from a point of its surplus, thus serving as grid energy storage, similar of even better than electricity. **The current status and perspective of hydrogen economy will be presented.** The convenient storage of hydrogen is the major challenge which, along with the lack of means of its cheap production, hampers the large-scale implementation of hydrogen economy. The main focus of this lecture will be made on chemical hydrogen storage media. They can be grouped into three main classes: the relatively heavy metal-based alloys, the light-weight chemicals which store hydrogen in a form of molecules or ions, and porous frameworks able to capture molecular hydrogen.

Metal-based alloys are limited by relatively low gravimetric hydrogen content. Nevertheless, they are already in a wide practical use, and are of special interest for stationary applications. Recent studies reveal a rich chemistry of metal-hydrogen interactions, which can not be rationalized by a geometrical model (localization of hydrogen atoms in voids of an appropriate size, taking account of repulsive H...H interactions), and suggest a directional bonding between metal and hydrogen atoms.

The light-weight hydrides (e.g. LiBH_4) contain hydrogen bound within stable anions and can produce large amounts of H_2 upon thermal decomposition (pyrolysis) or in a reaction with water (hydrolysis). Although considered as a main hope for the future of the hydrogen economy, these systems are commonly too stable for practical applications. On the contrary, absorption enthalpy of molecular hydrogen in **porous solids** is relatively low, and currently hydrogen can be stored in MOFs only at temperatures of liquid nitrogen.

Recent progress in materials for hydrogen storage will be reviewed, with an interesting insight into chemistry of hydrogen-rich solids. The need to break and form strong covalent bonds raises difficulties in the design of these truly "chemical" hydrogen storage systems. Advances in this area started with the discovery of catalysts for the reversible dehydrogenation of alanates [1], and this success inspired the research on even more sturdy borohydrides. A combination of different metals was used to tune the decomposition temperature in the wide range recently [2]. Also, formation of borohydride complexes has been recognized as a design principle, opening the door to the discovery of many new metal borohydrides. I will present design of light complex hydrides based on aluminium chemistry, where Al^{3+} serves as a template for H-conversion [3]. To achieve the ultimate goal of the reversible hydrogen storage using light complex hydrides, the reactive hydride composites (RHCs) have to be explored, considering many combinations of the high H-capacity materials [4].

[1] B. Bogdanovich, M. Schwickardi, *J. Alloys Compd.* **1997**, 254–256, 1.

[2] D. B. Ravnsbæk et al., *Angew. Chem. Int. Ed.* **2009**, 48, 6659.

[3] I. Dovgaliuk, Y. Filinchuk, *Int. J. Hydr. Energy* **2016**, 41, 15489.

[4] M. Paskevicius et al., *Chem. Soc. Rev.* **2017**, DOI: 10.1039/c6cs00705h