POROUS METAL HYDRIDES AS A PLATFORM FOR *IN SITU* STUDIES OF THERMODYNAMICS AND KINETICS OF GUEST UPTAKE

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Porous frameworks attract much attention as the potential materials for diffusion-controlled processes of selective guest adsorption and separation. High hydrogen uptake and separation of the molecules with a similar kinetic diameter belong to such challenging applications. The *in situ* monitoring of the accompanying structural changes sheds light on their adsorption and diffusion mechanisms. With respect to the possibility of observation of any behaviour regarding the guest molecules by the X-ray diffraction methods (e.g. powder X-ray diffraction, PXRD), the use of the light metal porous frameworks (e.g. hydride-based) results in a pronounced contrast between an empty and guest loaded framework structures.

Our interest is paid for selective capture and separation of chemically inert Kr and Xe [1] in nanoporous γ-$Mg(BH_4)_2$ [2]. Using advanced sub-second *in situ* PXRD, three diffusion scenario have been evaluated from the isothermal kinetics adsorption for a series of gases: Ar, Kr and Xe [3, 4]. The microscopic diffusion pathways and the activation barriers were rationalized from the macroscopic kinetic models and the crystal structure analysis. The lowest activation barrier has been estimated for the Ar atoms, which are smallest in the series. Consequently, these atoms equally easy diffuse through the intra- and interchannel apertures of γ-$Mg(BH_4)_2$ crystal structure [3, 4]. The diffusion of larger Kr atoms involves two activation energies: both intra- and interchannel barriers, which are higher than ones for Ar. Finally, the largest from the series Xe atoms diffuse only along 1-D channels with the highest activation barrier. The obtained kinetic characteristics are essential for the estimation of gas selectivity.

Therefore light metal hydride frameworks, can be used for sub-second PXRD which offers unique information on the energetics and microscopic mechanisms of diffusion not accessible in macroscopic gravimetric and volumetric methods.

References:

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Dr. Iurii Dovgaliuk spent his student's years in Chemistry Department of Lviv National Uviversity named Ivan Franko (Ukraine), which is well-known as one of the main crystallographic schools in Ukraine. During this time he obtained his first experience with X ray diffraction and crystallography.

After the Master degree graduation with honors, started his PhD thesis at Université catholique de Louvain (UCL, Belgium) in the young group of Prof. Y. Filinchuk. The main subject of his PhD thesis was devoted to the hydrogen storage. His new subject was focused on the synthesis and full characterization of new compounds and composites based on hydrogen-rich chemical and complex hydrides. The main attention was given to the new aluminum-based hydrides, investigated as potential materials for hydrogen storage upon their thermal decomposition.

Dr. Dovgaliuk continued his research carrier at the Swiss-Norvegian Beamlines (SNBL), which is located at the European Synchrotron Radiation Facility (ESRF, Grenoble), a few months after the PhD graduation. Here he changed his topic to in situ X-ray diffraction of gas adsorption by porous frameworks. During this post-doctoral research, he investigated the thermodynamics and kinetics of guest adsorption by porous frameworks, combining the phenomenological models and diffraction experiments.

Since 2019 have been working at the Institut des Matériaux Poreux de Paris (IMAP), where his scientific activity is focused on the investigation the crystal structure of novel metal organic frameworks (MOFs), as well as their gas adsorption using time-resolved in situ X-ray diffraction.

Education and scientific background:

- 2019 – present. Postdoctoral and research engineer positions at the Institut des Matériaux Poreux de Paris (IMAP) at ENS, Paris.
- 2016–2019 – Postdoctoral research at the Swiss-Norwegian Beamlines (SNBL) from the European Synchrotron Radiation Facility (ESRF in Grenoble, France); supervisor Dr. D. Chernyshov.
- 2011–2015 – PhD at the Institute of Condensed Matter and Nanosciences (IMCN), Université catholique de Louvain, Belgium; supervisors Profs. Y. Filinchuk and M. Devillers.
- 2010–2011 – Diploma of Master (with honour) in chemistry, Ivan Franko National University of Lviv, Ukraine; supervisor Prof. R. E. Gladyshevskii.
- 2006–2010 – Diploma of Bachelor in chemistry, Ivan Franko National University of Lviv, Ukraine; supervisor Dr. L. P. Romaka.