MS33-P05 | NOBLE GAS ADSORPTION IN MFU-4L FRAMEWORKS WITH DIFFERENT METAL ATOMS

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The detailed xenon/krypton gas adsorption and *in situ* X-ray powder diffraction measurements on seven different frameworks with MFU-4*l* structure [1] under different temperatures and pressures allowed following step-by-step the formation of the first and second adsorption layers in large and small cavities of these frameworks and identification of different structural factors favouring the noble gas adsorption through increasing the isosteric heat of adsorption, as well as precise interpretation of the shape of experimental adsorption isotherms.

Structural investigations revealed the sequence of filling of multiple adsorption sites (up to 10 crystallographycally independent positions) in two sequential adsorption layers and formation of quasi-solid structure by adsorbed Xe and Kr atoms (stabilised by van der Waals interaction) above their boiling temperature. The distances between adsorbed Xe or Kr atoms in the cavities are very close to the distances in the solid Xe and Kr, respectively. Our research also revealed that the pore geometry have a critical influence on the noble gas adsorption and can strongly influence the involvement of open metal sites and polarizable linkers into the process of Xe and Kr adsorption.

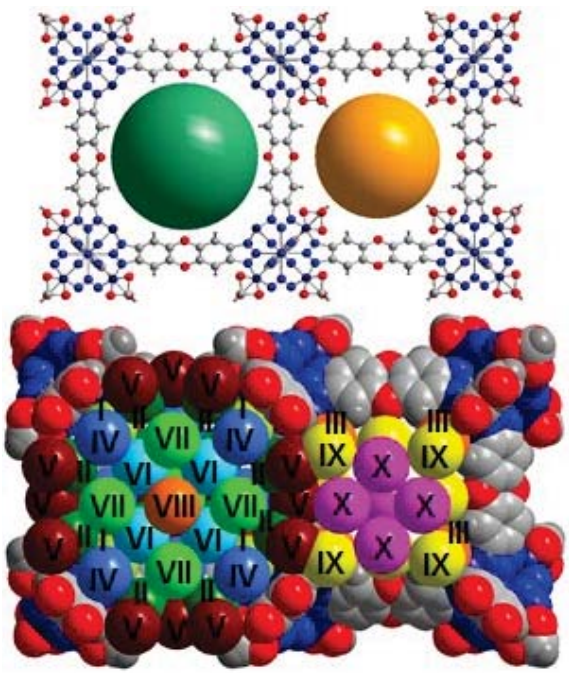

Fig. 1. (top) Crystal structure of MFU-4*l* framework with two types of alternating cavities: large and small cavities; (bottom) generalized structure of MFU-4*l* with all 10 positions of Xe atoms occupied (van der Waals radii for all atoms ; crystallographycally independent positions of Xe atoms are labelled from I to X).Unlabelled atoms : oxygen (red), nitrogen (blue), carbon and hydrogen (gray).

[1] D. Denysenko et al. *Chem. Eur. J.*, **17**, 1837 (2011)