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P06 Pronounced guest-guest interactions for argon in nanoporous γ-$Mg(BH_4)_2$ revealed by structural studies

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The physisorption of noble gas argon in γ-$Mg(BH_4)_2$ is investigated by in situ synchrotron X-ray powder diffraction. X-ray diffraction is an uncommon method for adsorption studies that gives more than just adsorption curves but also unequalled structural information useful to understand the adsorption mechanism. γ-$Mg(BH_4)_2$ is a nanoporous borohydride first discovered in our laboratory in 2011 (Filinchuk *et al.*, 2011). Its structure is an interesting framework of linked cavities, the size of approximatively two argon atoms, forming narrow porous channels with hydridic surfaces.

It is found that unexpected guest-guest interactions govern a reconstruction of the guest sublattice due to repulsions between guest molecules and the small pore size. Two distinct adsorption crystallographic sites exist, the most stable and first occupied at the centre of the porous cavity, and the second closer to the pore aperture. After a first saturation, that is observable on the adsorption curve, the adsorption of a second Ar atom leads to the occupation and displacement of the second crystallographic site, decreasing repulsive interactions between guest molecules, allowing two argon atoms to adsorb per pore and the observation of a second adsorption curve.

The collection of two different isobars allows to calculate the isosteric heat of adsorption by the Clausius-Clapeyron relation up to the first saturation. Argon isosteric heat of adsorption ranges from 16.0 kJ/mol for the empty phase to 10.5 kJ/mol for the loaded phase. The variation on the isosteric heat of adsorption is explained by the guest-guest interaction.

Some comparisons are made with preliminary krypton and xenon adsorption experiments in γ-$Mg(BH_4)_2$.

Reference
Filinchuk, Y., Richter, B., Jensen, T. R., Dmitriev, V., Chernyshov, D. & Hagemann, H. (2011). *Angew. Chemie - Int. Ed.* **50**, 11162–11166.