

Invitation à la soutenance publique de thèse

Pour l'obtention du grade de Docteur en Sciences

Monsieur Fabrice MORELLE

Master en sciences chimiques à finalité approfondie

Hybrid hydridic frameworks by the combination of complex hydrides and nitrogen-based organic ligands

Over the past 15 years, the research in hydrogen storage and the advances in powder diffraction techniques led to the discovery and structural characterization of numerous metal borohydride ($M_a(BH_4)_b$) revealing bonding schemes similar to those of metal-organic-frameworks, the borohydride anion behaving as the linker.

In this work, we combined metal borohydrides with neutral and negatively charged nitrogen-based organic ligands searching for hybrid compounds containing both the hydridic borohydride anion and the organic moiety in a single structure. This strategy was aiming at the formation of a new class of porous materials in which the organic part would provide the structural rigidity and the borohydride would provide the functionality. Mechanochemistry, a method in which solids are directly combined without or with very small amounts of solvent, was the most used synthetic tool throughout the work.

The focus was placed on the structural characterization of the compounds. Neutron powder diffraction and *ab initio* calculation were used to complement the synchrotron radiation X-ray powder diffraction data when the latter were not sufficient to build satisfactory structural models. Other techniques were used to probe the properties suggested by the structural features of the obtained materials.

The compounds prepared showed that the structures are dominated by the interaction between the organic ligand and the metal, the borohydride group accommodating unfavorable coordination environments in some cases. This brings to the conclusion that despite its structure directing tendency, the borohydride group is not the suitable building block for the construction of porous hybrid compounds. However, this unfavorable environment leads to unprecedented rotational dynamics of the BH_4 group with possible rotational tunneling.

Mardi 7 novembre 2017 à
16h15

Auditoire SUD 08
Croix du Sud
1348 Louvain-la-Neuve



Membres du jury :

Prof. Yaroslav Filinchuk (UCL), promoteur

Prof. Eric Gaigneaux (UCL), président

Prof. Michaël Singleton (UCL), secrétaire

Prof. Michel Devillers (UCL)

Dr. Michaël Felderhoff (Max-Planck-Institut für Kohlenforschung, Germany)