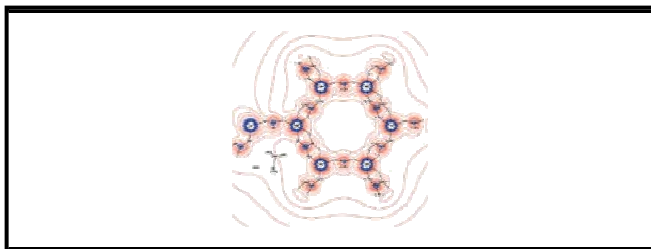


chemistry etc. We focused our attention to metal oxalates, testing the possibility to model electron density of building blocks and obtain at least approximate evaluation of the properties.

In these materials, the oxalate ion often acts as a rigid bidentate ligand which bridge metal centres [2] therefore facilitate the formation of extended structures with dimensionalities ranging from zero to three [3].

New inorganic-organic hybrid structures based on Zinc oxalate structures, which show 1D linear, 2D honeycomb and 3D structures were studied. In order to model the building blocks of these frameworks, we used as benchmark some simple structures like $Zn(C_2O_4)$, $Zn(C_2O_4)(H_2O)$, $Zn(C_2O_4)(C_4N_2H_{10})$, $(HC_2O_4)_2(C_4N_2H_{12})$. All compounds were obtained through hydrothermal synthesis. Electron density distribution was studied through X-Ray diffraction and through density functional theory.

Once the modelling was refined and tested, the electron densities of 1D-2D-3D framework were computed using multipoles restricted to optimized theoretical building blocks. This allows to reconstruct the electron density of more complex structures, often not available in the form of good quality single crystals. The results are utilised for evaluation of material properties such as electrostatic potential (a Zn oxalate honeycomb is plotted in the Figure), the interaction energies between the framework and neutral guest molecules or counter-ions, and the calculation of the active surface areas of the framework [4].



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Keywords: Zinc Oxalates, Electron Density, X-Ray Diffraction, Metal Organic Frameworks

L.A.31

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Formation of $2NaBH_4/MgH_2$ system from $2NaH/MgB_2$ by hydrogenation

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Borohydrides with a general formula MBH_4 (where M stands for an alkali or an alkali earth metal) are considered as prospective hydrogen storage materials due to a high percentage of hydrogen (up to 20 wt%) [1].

An interesting complex hydride for hydrogen storage is sodium tetraborohydride ($M = Na$). $NaBH_4$ desorbs hydrogen easily [2] but the reversible reaction requires very strong conditions (550 – 700 °C and 30 – 150 bar H_2) [3]. It was found that MgB_2 can facilitate the reversibility reaction [4]. It was shown that formation of $NaBH_4$ does not occur directly, but follows the formation of $MgNaH_3$. But it seems that reaction mechanism strongly depends on the conditions of experiment.

In order to find out the optimal conditions of formation of $2NaBH_4-MgH_2$ system from $2NaH-MgB_2$ and to understand better the reaction mechanism, several experiments were performed. Hydrogen absorption by starting ball-milled compounds ($2NaH-$

MgB_2) was studied at isotherm conditions at several temperatures (400, 425, 450 °C) at 100 bar H_2 pressure. Experiments were performed *in-situ* using synchrotron radiation.

The results indicate different way of $NaBH_4$ and side products formation depending of temperature and hydrogen pressure. Further experimental results will be presented to discuss the optimal conditions for hydrogen absorption in the indicated system.

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Structural studies of the RNA polymerase III transcription factor IIIC

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Transcription in eukaryotes is divided over three different RNA polymerases, termed RNA polymerase (Pol) I, II and III, which have different target genes. Pol III is the most complex of these three polymerases consisting of 17 different subunits compared to 12 and 14 for Pol II and Pol I, respectively. However, the process of polymerase recruitment and transcription initiation in the Pol III system is arguably less complex, especially when compared to Pol II. On most Pol III-transcribed genes, two transcription factors are sufficient to recruit the polymerase (Schramm and Hernandez, 2002). These are known as the RNA polymerase III transcription factors IIIB and IIIC (TFIIIB and TFIIC). On these type 2 (e.g. tRNA) genes, TFIIC gets recruited to the gene-internal B-box through a very strong interaction, followed by binding of this transcription factor to the A-box. Subsequently, promoter-bound TFIIC recruits TFIIIB, and the TFIIIB-TFIIC-DNA complex recruits the polymerase, after which transcription can initiate. We have determined several crystal structures of various parts of TFIIC, and have performed electron microscopy studies of the whole transcription factor.

Schramm, L., and Hernandez, N. (2002). Recruitment of RNA polymerase III to its target promoters. *Genes Dev* 16, 2593-2620.

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