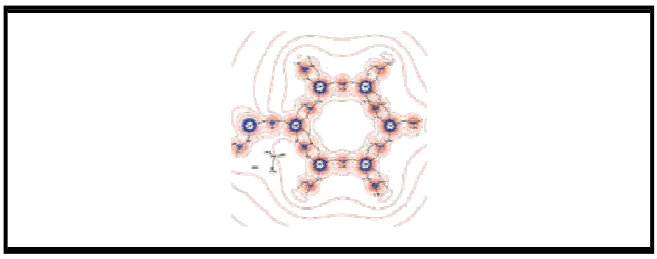
chemistry etc. We focused our attention to metal oxalates, testing the possibility to model electron density of building blocks and obtain at least approximate evaluation of the properties.

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 NaBH4 does not occur directly, but follows the formation of MgNaH3. 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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Keywords: hydrogen storage, borohydrides, diffraction

L.A.32

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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 TFIIIC). On these type 2 (e.g. tRNA) genes, TFIIIC 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 TFIIIC recruits TFIIB, and the TFIIIB-TFIIIC-DNA complex recruits the polymerase, after which transcription can initiate. We have determined several crystal structures of various parts of TFIIIC, 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.

L.A.33

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Viva Biotech Ltd. -- Protein Expert for Drug Discovery

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Viva Biotech, headquartered in the pharma-valley of Shanghai, China, is a premium preclinical drug discovery service provider to pharmaceutical and biotech companies worldwide. Viva is privately owned and financed by a leading US private equity fund. It currently employs 200 scientists working in a state-of-the-art research center spanning 65,000 square feet. The research center includes cell culture/biochemistry/crystallography laboratories, medicinal chemistry/bioanalytical laboratories, and animal facilities.

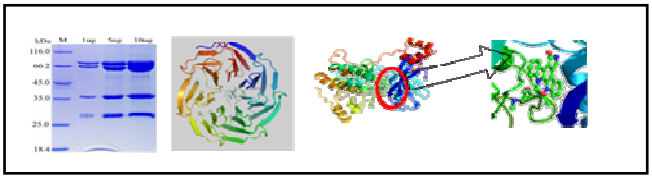
Viva is one of the very few CROs that integrate those technologies with X-RAY, MS, NMR and SPR platform, thereby providing a full line of drug discovery services to pharmaceutical and biotech companies. With this integrated technology platform, Viva's scientists team has involved in the preparation of several hundreds of drug targets and determined several hundreds of crystal structures every year to most of big pharmaceutical companies as well as dozens of biotech companies.

Viva has taken the protein and structure services to a new height by successfully providing GPCR protein crystallography to clients.

Building on the success of the aforementioned gene-to-protein and gene-to-structure services, Viva has expanded services to the structure-based drug discovery with strong in-house capabilities in medicinal chemistry and computational chemistry. With the addition of antibody research, bioanalytical and in vivo pharmacology platforms, Viva is well positioned to provide an integrated drug discovery service capable of executing from hit generation to lead optimization programs for clients.

In summary, Viva has expertise and large technical base in each of the following areas:

1. Gene-2-structure and gene-2-protein with preparation of several thousands of proteins and several hundreds of crystal structures each year, and with world class expertise in GPCR protein crystallography.
2. Structure-based drug discovery (hit generation to lead optimization)
3. Unmatched experience and expertise in biophysics techniques including: X-ray, NMR, MS, and SPR
4. High-level medicinal chemistry
5. Fragment-based drug discovery preclinic structure-based drug discovery (hit generation to lead optimization)
6. Antibody research platform with phage display library
7. In vivo disease models in CNS, oncology and inflammation



L.A.34

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The molecular weight of proteins from a single SAXS measurement on a relative scale

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An important step in the characterization of proteins is the determination of their molecular weights and their multimeric state in solution. Accuracies of classical methodologies for the determination of the molecular weight of proteins in dilute solution were recently evaluated by Mylonas & Svergun [1]. These authors demostrate that the molecular weight of a protein can be obtained by comparing the experimental SAXS curve produced by the protein in dilute solution *(i)* to another experimental SAXS curve corresponding to a standard protein with known molecular weight, or *(ii)* to a SAXS curve corresponding to pure water leading in this case to the determination of SAXS intensity of the studied protein in an absolute scale. Both of these procedures require the determination of at least two SAXS curves. In addition, the first procedure requires the precise knowledge of the protein concentration, which is frequently not known with high accuracy, and the second method needs the determination of the SAXS intensity by water with a considerable precision, which implies in rather long counting times. Both methodologies yield the molecular weight of proteins with an error of about 10% provided the solute concentration is measured with an accuracy of 5 – 10 %, which might not always be straightforward. A novel procedure for the determination of the molecular weight of proteins in diluted solution from a single SAXS curve measured on a relative scale is avaiable, which uses experimental data of a single small angle X-ray scattering (SAXS) curve measured on a relative scale [2]. This procedure does not require the measurement of SAXS intensity on an absolute scale and does not involve a comparison with another SAXS curve determined from a known standard protein. The proposed procedure can be applied to monodisperse systems of proteins in dilute solution, either in monomeric or multimeric state, and it was successfully tested by applying it to SAXS data measured for 22 proteins with known molecular weights. The molecular weights determined by using this novel method of all the measured set deviate from their known values by less than 10 % and the average discrepancy was 5.6 %. Importantly, this method allows for a simple and unambiguous determination of the multimeric state of proteins with known monomeric molecular weight.

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Keywords: SAXS, Protein, Molecular weight

L.A.35

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Parallel alignment interactions of water and aryl rings at large displacements

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Water plays an essential role in nature. Its geometry, small size, and high polarity govern its capabilities and the complexity of its behavior. Most important is its ability to form strong hydrogen bonds with polar molecules and builds strong networks with itself. In addition to these strong intermolecular interactions, water molecules also have important weaker interactions with less polar molecule. The water–benzene complex has been the subject of extensive investigation.

Recently, we recognized the parallel alignment interactions of water and aromatic rings [1]. These important new geometric features were discovered by examining crystal structures from the Cambridge Structural Database (CSD) and analyzed by ab initio calculations of the water–benzene dimer including coupled cluster electron correlation treatment (CCSD(T)) and complete basis set extrapolation.

Analysis of crystal structures from the Cambridge Structural Database (CSD) revealed the existence of orientation where the whole water molecule (A set) or one of its O–H bonds (B set) is