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<table>
<thead>
<tr>
<th>TIME</th>
<th>MONDAY</th>
<th>TUESDAY</th>
<th>WEDNESDAY</th>
<th>THURSDAY</th>
<th>FRIDAY</th>
</tr>
</thead>
<tbody>
<tr>
<td>9-9.45</td>
<td>Neutron facilities at the BNC</td>
<td>Lecture</td>
<td>Lecture</td>
<td>Lecture</td>
<td>Lecture</td>
</tr>
<tr>
<td>9.45-10</td>
<td>L. Rosta</td>
<td>TOF</td>
<td>M. Russina</td>
<td>G. Kreiner</td>
<td>Practical work at spectrometers by groups</td>
</tr>
<tr>
<td>10-10.45</td>
<td>Lecture</td>
<td>Radiation protection</td>
<td>Neutron diffraction</td>
<td>Introduction to neutron reflectometry</td>
<td>Practical work at spectrometers by groups</td>
</tr>
<tr>
<td>10.45-11</td>
<td>A. Szakal</td>
<td>A. Len</td>
<td>E. Oksanen</td>
<td>M. Avdeev</td>
<td>Practical work at spectrometers by groups</td>
</tr>
<tr>
<td>11-11.45</td>
<td>Lecture</td>
<td>Lecture</td>
<td>Lecture</td>
<td>Lecture</td>
<td>Lecture</td>
</tr>
<tr>
<td>11.45-12</td>
<td>Neutron radiography</td>
<td>Neutron radiography</td>
<td>Prompt Gamma Activation Analysis</td>
<td>Imaging and elemental analysis of porous materials</td>
<td>Practical work at spectrometers by groups</td>
</tr>
<tr>
<td>12-12.14</td>
<td>L. Szentmiklósi</td>
<td>L. Szentmiklósi</td>
<td>L. Szentmiklósi</td>
<td>V. Szinger Szilágyi</td>
<td>Practical work at spectrometers by groups</td>
</tr>
<tr>
<td>12.14-14</td>
<td>Lunch</td>
<td>Lunch</td>
<td>Lunch</td>
<td>Lunch</td>
<td>Lunch</td>
</tr>
<tr>
<td>14-14.45</td>
<td>Lecture</td>
<td>Lecture</td>
<td>Lecture</td>
<td>Lecture</td>
<td>Lecture</td>
</tr>
<tr>
<td>14.45-15</td>
<td>Introduction to SANS</td>
<td>2D SANS</td>
<td>2D SANS</td>
<td>2D SANS</td>
<td>Lecture</td>
</tr>
<tr>
<td>15.16-19</td>
<td>14-17 Practical work at spectrometers by groups</td>
<td>14-17 Practical work at spectrometers by groups</td>
<td>14-17 Practical work at spectrometers by groups</td>
<td>14-17 Practical work at spectrometers by groups</td>
<td>14-17 Practical work at spectrometers by groups</td>
</tr>
<tr>
<td>19-21</td>
<td>Welcome reception and poster session</td>
<td>Welcome reception and poster session</td>
<td>Welcome reception and poster session</td>
<td>Welcome reception and poster session</td>
<td>Welcome reception and poster session</td>
</tr>
</tbody>
</table>
Among the objects of the study of modern physics of condensed matter, occupy a special place compounds and materials based on iron oxides with a structural type of perovskite. These materials have a wide range of crystal and magnetic properties depending on the degree of doping, temperature or high pressures. One of the interesting properties of the oxides PbFe\(_{0.5}\)Sb\(_{0.5}\)O\(_3\) and PbFe\(_{0.5}\)Nb\(_{0.5}\)O\(_3\) are the order and disorder of the magnetic and paramagnetic ions in the crystal cell. This fact strongly affects the magnetic properties that determine the unique magnetic structures: from ferromagnetic to disproportionate.

The report presents the results of the study of crystal and magnetic structures of iron oxides with a structural type of perovskite of nominal composition: PbFe\(_{0.5}\)Sb\(_{0.5}\)O\(_3\) and PbFe\(_{0.5}\)Nb\(_{0.5}\)O\(_3\) in a wide temperature range using neutron diffraction, which were carried out using the DN-6 diffractometer of the reactor with a high pulse flow IBR-2 at JINR, the Laboratory of neutron physics. I. M. Frank.

Crystal structure of ordered perovskite PbFe\(_{0.5}\)Sb\(_{0.5}\)O\(_3\) is described by the tetragonal symmetry I\(_4\)/m, in which iron and tin atoms alternate. At low temperature, the appearance of magnetic reflexes is observed, which correspond to the antiferromagnetic ordering with the propagation vector \(k = [\frac{1}{2}, \frac{1}{2}, 0]\). The structural mechanisms of the formation of this magnetic state are discussed.

In disordered perovskite, PbFe\(_{0.5}\)Sb\(_{0.5}\)O\(_3\) the appearance of g-type antiferromagnetic ordering at low temperatures is observed. The report presents the parameters of the crystal lattice, bond length, magnetic moments of iron for this compound, the models of crystal and magnetic structures based on these data.
The dependence of polyurethane microparticles’ surface charge on the solvent pH

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The use of different polymers as drug delivery systems has increased enormously in recent years. Polyurethane materials have many uses: they are often found as foams in the automotive industry, as thermal insulation panels in refrigerators and in the walls of buildings, as elastomers used in footwear, as injection moulded components for various industrial applications. Their biocompatibility and biodegradability have been demonstrated long time ago, before they were patented as wound dressings, catheter tubing, surgical drains, intra-aortic balloon pumps, dialysis devices, etc. [1]

We optimized the synthesis of the polyurethane drug carriers and we obtained a very wide range of particles’ size (between 80 and 4000 nm) in the last 8 years. The thermal behaviour of these particles was assessed by DSC technique and a very good stability was observed up to 300 °C. The encapsulation efficacy and the drug release rate were evaluated by UV-VIS spectrometry for different herbal extracts, and the results were calculated by Beer-Lambert law. SANS method was involved to determine the textural properties of these particles [2] and almost identical values of the fractal dimensions between the empty polyurethane particles and the particles containing a chili pepper extract were found by the Yellow Submarine and FSANS instruments at Budapest Research Reactor (Hungary).
The aim of this study is to understand the mechanism of these microparticles’ surface charge by measure their Zeta potential at different pH values.

Figure 1. Input and output values panel of a Wallis analyzer by Cordouan Technol. (France)

Perspectives

In the present study, an inverse correlation between the polyurethane microparticles’ surface charge and the solvent pH was found and this is probably due to the deprotonation of the -NH- groups from the polyurethanes. New correlations between the particles’ surface charges and their fractal dimensions are very interesting to be studied.

References
[2] Borcan LC; Dudas Z; Len A; Fuzi J; Borcan F; Tomescu MC. Int J Nanomed., 2018, 13, 7155-7166
Structural flexibility of thylakoid membranes revealed by small-angle neutron scattering

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Biological organisms capable of oxygenic photosynthesis developed highly organised structures to convert light energy into chemical energy. Small-angle neutron scattering (SANS) is a non-invasive technique, free of radiation damage – ideally suited for characterising complex biological macro-assemblies on the mesoscopic scale. Earlier SANS measurements have provided statistically and spatially averaged information about the structure of multilamellar thylakoid membrane systems in different photosynthetic organisms. SANS has also revealed light-induced reversible structural changes on a time scale of seconds to minutes - small but well discernible variations in the characteristic repeat distances of the thylakoid membranes in isolated chloroplasts, living unicellular organisms and intact leaves. Some of these reorganisations have been shown to be associated with key regulatory mechanisms of photosynthesis. In my poster presentation I will summarize the present state of this field, and outline my proposed contribution to better understand the nature of thylakoid membrane reorganisations elicited by different biotic and abiotic stress conditions in algae and plants.
Discovering exotic magnetism due to competing magnetic interactions in layered perovskites with 3d hetero-species B-site ions has remained an intriguing topic with many unexplained features. Here we study Exchange bias (EB) phenomena in a single-layered Ruddlesden-Popper SrLaCo$_{0.5}$Mn$_{0.5}$O$_4$ using state of the art measurement such as susceptibility, neutron diffraction, and training effect along with density functional calculations. EB as large as ~5.5 kOe is observed in SrLaCo$_{0.5}$Mn$_{0.5}$O$_4$ which is the highest ever found in any layered transition metal oxides including Ruddlesden-Popper series. Neutron diffraction measurements and together with dc magnetic measurements suggest the formation of short-range magnetic domains. By carrying out density functional calculations on several model configurations, we propose that EB is originated at the boundary between Mn-rich antiferromagnetic and Co-rich ferromagnetic domains at the sub-nanoscale. Our analysis infers that the presence of competing magnetic interactions is sufficient to induce exchange bias and thereby a wide range of materials exhibiting EB can be engineered.
Physical activity in remodeling bone alterations produced by secondary osteoporosis in rats


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Osteoporosis is a condition resulting in an increased risk of skeletal fractures due to a reduction of bone-mass and micro-architectural deterioration of the tissue. Aside from postmenopausal osteoporosis, the most common secondary cause of this disease is due to the long-term use of oral glucocorticoids, a common cure for many inflammation diseases.

The most significant mechanism of glucocorticoid-induced osteoporosis in enhanced bone resorption and decreased bone formation. [1]

The exposure to glucocorticoids leads to a depletion of osteoblast lineage accompanied by osteoblast apoptosis, but also shifting the differentiation of pluripotent stromal cells away from osteoblast and toward the adipocyte lineage. [2]

The present study was designed to illustrate the benefit of physical activity, an inexpensive and accessible treatment, in the amelioration of osteoporosis symptoms.

Animals (adult female Wistar rats) were divided into four groups: control, control with a daily swimming session, glucocorticoid-treated (daily dose 0.4 mg/kg b.wt.), and glucocorticoid-treated performing a daily swimming session. The experiment had a duration of one month.

Hematological parameters related to bone function were assessed, together with markers of membrane integrity, and activities of certain antioxidant enzymes. Elemental microanalysis of the cortical thigh-bone was done with the EDX (Energy Dispersive X-Ray) system.
For a better understanding of the structural parameters, inside the bone structure, the samples were measured using the small-angle neutron scattering (SANS) spectrometer YuMO, IBR-2 reactor, at Frank Laboratory of Neutron Physics, from Joint Institute for Nuclear Research, Dubna, Russia.

Membranes permeability, as indicated by activities of ALT, AST and LDH in serum and tissues, showed no changes in the liver and skeletal muscle cells, while myocardial cells seemed to release ALAT under the effects of glucocorticoids.

Glucocorticoid treatment reduced calcium concentration in the cortical bone with 64% and phosphorus concentration with 51%, as compared to the control group. The physical activity in the glucocorticoid + effort group showed a marked tendency of restoration of these parameters.

Figure 1. Active comparison of SANS spectra from the first three groups without the bone 4 influence. Bone 1 – control animal; bone 2 – control with effort animal; bone 3 – glucocorticoid animal; bone 4 – glucocorticoid with effort animal.

Figure 2. SANS data on bone 1 and bone 4 structural comparison. Bone 1 – control animal; bone 4 – glucocorticoid with effort animal.

SANS measurements confirmed the deterioration of the bone structure, in the group that received glucocorticoids (Figure 1, red circles). The
control group that performed physical training (Figure 1, blue circles) showed an improved bone density, as compared to the control sedentary animals. Bone tissue density of the glucocorticoid + effort group (Figure 2, green) was close to that of the control group. We may conclude that physical activity helps consolidating the bone structure.

References:
Defect Chemistry Investigations on Doped PbTiO$_3$ Perovskites Used in Solar Energy Conversion

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Solar energy storage in chemical bonds is one of the major challenges to provide a sustainable technology for this renewable energy source. Hence, due to its energy demand, the elimination of oxygen in solar thermochemical and photocatalytic applications is the most critical step to overcome. At this point, transition metal doped perovskites emerge as potentially promising candidates based on thermodynamic analysis of oxygen vacancy formation. Among different perovskite materials, PbTiO$_3$ is known to be a good visible light photocatalyst, acting as an oxidizer. In this study, the effect of Co$^{2+}$ and Cu$^{2+}$ doping on PbTiO$_3$ perovskite was investigated in means of oxygen vacancy formation and band gap changes via spectroscopic methods. Undoped and doped PbTiO$_3$ materials were synthesized through sol-gel method and their structures will be analyzed with XRD, UV-Visible Diffuse Reflectance and EPR Spectroscopy. The perovskite structure was verified via XRD measurements for all synthesized materials. According to preliminary X-Band EPR measurements, incorporation of Co$^{2+}$ in the perovskite on Ti$^{4+}$ site was detected. Hence an oxygen vacancy accompanying this substitution will be favorable to provide lattice charge balance. Moreover, preliminary UV-VIS diffuse reflectance spectroscopy measurements indicated that addition of cobalt enhanced absorption in the visible region and increase in the band gaps. The changes in band gaps can be explained by changes in oxygen vacancy concentration which can be attributed to Co$^{2+}$ doping amount. For Cu$^{2+}$ doped materials, a semi-empirical approach that estimates oxygen vacancy type with EPR results will be presented as well.
Potential small angle neutron scattering application for determination of the size, aggregation number and the shape of the aggregates of sodium isoursodeoxycholate and sodium isoehenodeoxycholate aggregates in water

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Bile salts form hydrophobic Small’s primary micelles at concentrations above the critical micelle concentration (CMC), while at concentrations above 3CMC they form secondary micelles (by the association of primary micelles via H-bonds). Thermodynamic functions of the self-association of the anions of isoehenodeoxycholic acid (3-epimer of henodeoxycholic acid, ICD) and the anions of isoursodeoxycholic acid (3-epimer of ursodeoxycholic acid, IUD) is examined, and formation of IUD aggregates with two or three building units is slightly more favorable via α sides of steroid skeletons, regarding hydrophobicity, while regarding steric repulsive interactions it is more favorable to associate via β sides. Due to this, IUD in the vicinity of the CMC can form primary micelles by association of IUD particles both from the convex side and from the concave side of the steroid ring system. Therefore, IUD is significantly more prone to initial micellization than bile salt derivatives whose steroidal skeletons contain equatorially oriented OH groups.
SANS study of cycloidal magnetic domains in multiferroic BiFeO$_3$

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Despite the high interest in BiFeO$_3$, which is the most studied multiferroic compound due to its room-temperature multiferroic phase, a detailed study of the magnetic domain structure of the material is not yet performed. Motivated by the THz absorption measurements of our group I carried out small-angle neutron scattering (SANS) experiments to observe the magnetic field dependency of the domain structure. In contrast to the common belief not just the populations of the cycloidal domains change with the magnetic field, but also the q vectors are rotated. The reorientation of the modulation vectors are driven by the larger out-of-plane susceptibility of the cycloids, thus, the q vectors are tend to be perpendicular to the direction of the external magnetic field.
Structural properties of TEMPO-oxidized nanocellulose hydrogels for biomedical applications

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The high availability, low cost and good biocompatibility make cellulose a widely employed starting material for a high numbers of applications. Recently nano dimensioned cellulose fibers (CNF) were subjected to a deep investigation and resulted to be versatile in many preparations. CNF can be easily prepared by a regioselective oxidation of the primary hydroxyls of cellulose to corresponding carboxylic groups, catalysed by TEMPO in the presence of NaBr/NaClO oxidizing system (TOCNF). [1,2] Depending on the concentration, aqueous dispersions of the TOCNFs may exhibit interesting rheological properties going from transparent, low viscous solutions to opalescent and highly viscous gels (see Figure 1). [3] In spite of this “gel-like” character, the structure can be easily disrupted by high shear rate to form a liquid due to its shear thinning character. Indeed, TOCNF dispersions’ behaviour can change reversibly between elastic-dominated and viscous-dominated regimes, a behaviour typical of thixotropic materials. [4] These thixotropic behaviours made these dispersion promising for different biomedical purposes, like injectable gels. Furthermore, the addition of electrolytes (e.g. Mg$^{2+}$, Ca$^{2+}$) into TOCNF dispersions enables to form homogeneous and stable hydrogels. The sol-gel transition is driven by the screening of superficial charges, due to the presence of carboxylates, which provide interfibril repulsion. This screening effect, leads to the reduction of interfibril distance and, in cases of metal ions with high valency (at least major than 1) to the cross-linking between fibrils (figure 2). In summary, the great capability of TOCNFs to form hydrogels with a good mechanical stability and the good biocompatibility makes them promising candidates for tissue engineering and biomedical applications in general. In this regard, many examples of biomedical applications of CNFs hydrogels, including those obtained by the TEMPO-mediated protocol, are reported in literature. These examples ranges from controlled drug release, [5] to covalently attach fibronectin to CNF hydrogel to enhance fibroblast
adhesion, [6] to the preparation of macroporous hydrogel scaffold supports to growing mouse fibroblast cells. [7]

Thanks to the support of CERIC and ELETTRA actions a multi-technique investigation of these system currently in progress. The main goal is to investigate, at microscopic and molecular level, the sol-gel transition observed in aqueous solutions of TOCNF in the presence of polyvalent cations, as a function of pH and temperature that are the parameters able to drive and regulate this characteristic transition phase in this system. We are collecting the information that can be extracted by exploiting the combined use of UV Raman scattering technique that is sensitive to intra- and inter-molecular interactions through the measurements of molecular vibrations, and the information on the structural organization offered by the use of small angle neutron scattering techniques, SANS.

By UV Raman spectroscopy we studied the OH stretching signal of water, well visible in the high frequency region of the UV Raman spectra of TOCNF gels, which is a probe of the structural rearrangement of hydrogen-bond network of water confined in the gel matrix. Moreover, small angles neutron scattering experiments have been recently carried out, with the main aim to clarify the main structural features of cellulose gels as a function of different experimental parameters. Brillouin lights scattering experiments have been also performed for a viscoelastic characterization of the cellulose gels. Overall these multi-technique measurements are expected to provide a comprehensive characterization of the cellulose matrices, which is a fundamental pre-required step for further applications.

Since we propose these hydrogels for biomedical application we are also investigating the effect of the loading in TOCNFs based hydrogels on the structure and stability of a model protein. To this aim, UV Resonant Raman (UVRR) spectroscopy were used for selectively enhancing specific vibration in particular regions of the biomolecule. In more detail, we explore two different excitation wavelengths in order to investigate the spectra where it is completely dominated by Tyrosine (tyr) and Tryptophan (trp) aromatic ring side-chain vibrations and where most of the contribution is expected to arise from peptide bond amide vibrations. By probing the different chromophoric segments of the biomolecule we are able to obtain detailed information on the secondary structure of lysozyme and the interaction with the environment at the different environmental conditions.
Figure 1: Aqueous dispersions of TEMPO-CNFS at different concentration. Indigotine dye was added to improve the visualization.

Figure 2: Scheme for the preparation of TOCNFs hydrogel cross-linked with CaCl$_2$

Figure 3: Final gel composed by addition of Ca$^{2+}$ to TOCNFs solution. Indigotine dye was added to improve the visualization

References:
Vortex Formation in \((\text{Ho}(1-x)\text{Er}x)\text{Ni}_2\text{B}_2\text{C}\)

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In order to study the vortex scattering and magnetic modulations on the magnetic superconductor samples \(\text{HoNi}_2\text{B}_2\text{C}_2\) and \(\text{ErNi}_2\text{B}_2\text{C}_2\) and their internal dopings, we grew single crystals of these structures. \(\text{RNi}_2\text{B}_2\text{C}\) is a material whose anti-ferromagnetic (AFM) and ferromagnetic (FM) phases coincide with superconductivity and hence the magnetic modulations are rich. Different type long-range order (LRO) to short-range order (SRO) of commensurate and incommensurate modulations make this system still interesting to be studied even today. Our samples are \((\text{Er}(1-x)-\text{Ho}x)\text{Ni}_2\text{B}_2\text{C}\) ranging from pure Er to pure Ho with increasing steps of \(x=25\%\) step size. The magnetization studies on these crystals are given in Fig.1. The superconducting temperatures (\(T_c\)) are \(T_c \approx 10\text{ K}\) which are more or less in the expected range for these materials. As Er amount increases in the samples, the \(T_c\) obtained under \(H\) decreases to the vicinity of \(T \approx 5\text{ K}\) where reentrance is completed. As it also can be seen, the FC and ZFC values are different. This difference is more pronounced for the doped samples. The difference of FC and ZFC could be explained with the idea of having some trapped fields in the samples, this makes it even more interesting since the same difference is not so large for the pure samples. For the pure samples, the Meissner effect is almost completed in both cooling ways. Therefore, they show superconductivity. The AFM reentrance behavior for pure Ho can also be seen from these data. We are in the process of doing SANS and elastic magnetic scattering measurements at this moment.
Figure 1 MPMS measurements on (Er-Ho)Ni$_2$B$_2$C single crystals. The magnetic field directions are given on the titles of each graph along the surface of samples. The mass of the samples are ranging from 10 mg to 20 mg. The reentrant AFM behavior is observed for pure Ho sample as the kink of the magnetization at $T \sim 5$ K. $T_c \sim 10$K values are in the expected range for these compounds.
Starting from a hybrid xerogel sample obtained by one-pot sol-gel method, a series of six nanocomposites of Fe$_2$O$_3$-SiO$_2$ were formed. The used precursors were: tetraethilortosilicate(TEOS), distilled water, polyvinyl alcohol (PVA), iron (III) acetylacetonate (Fe(acac)$_3$), methanol (MeOH) and nitric acid (HNO$_3$). The reactant mole ratio was: TEOS: H$_2$O: PVA: Fe(acac)$_3$: MeOH : HNO$_3$ = 1 : 10 : 0.63*10$^{-5}$ : 0.14 : 18 : 0.01. The six samples were obtained by thermal treatment at different temperature, specifically 180, 220, 260, 300, 400 and 500 °C. The used techniques for physicochemical characterization were: TGA, FTIR, EDAX, BET, SEM, TEM, XRD, Mossbauer and magnetic measurements. Based on our results we observed that at 220 °C the first changes in structures take place, presenting the maghemite specific structure. At this temperature a slight nanostructuration of the material could be noticed with the dimension around 5 nm with quite a low polydispersity. Further, by raising the temperature a transformation of maghemite into hematite was observed which take place at 400 °C. At this temperature the polydispersity of the particles in the aggregates tend to diminish and tend to average sizes around 30 nm. The materials obtained present superparamagnetic behavior.
The morphology of the structure of biodegradated bacterial cellulose

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Bacterial cellulose (BC) is synthesized by the bacterium *Gluconoacetobacter xylinum* on the surface of the growth medium in stationary conditions in the form of a dense film capable of holding a large amount of liquid in a ratio of 1: 100 (dry matter: water) and maintain high mechanical tensile strength [2]. Physico-chemical properties and the unique structure of the nano-gel film (NGP) of bacterial cellulose determine its widespread use in the creation of new composite materials for surgery, medicine and other areas [3]. It is known that with the use of traditional medical devices for treating various wounds, frequent change of dressing material entails injury to their surfaces [1]. Using the same BC as a wound dressing, which requires hygroscopicity, water and vapor permeability material, mechanical strength and biocompatibility, is a promising alternative to standard therapy. However, one of the significant limitations The use of BC biofilms for treating wounds is their low resorption due to the lack of cellulolytic enzymes in the human body.

The purpose of this work was to study the process of degradation of cellulose nano-gel cellobiohydrolase films from *Scytalidium candidum 3C* fungus, choice conditions of biodegradation of BC and conducting an in vivo experiment. Comprehensive analysis of raster microscopy data, low-temperature nitrogen adsorption and small-angle neutron scattering showed that the biodegradation of BC, catalyzed by cellobiohydrolase from *S. candidum 3C*, results in: 1. By increasing the thickness of the primary structural elements of the lamellar type, from which BC fibers are formed; 2. To reduce the specific area the surface of SBET (about 5–10%) of bacterial cellulose dried under supercritical conditions using CO2; 3. To loosen structures formed fibers of bacterial cellulose, and the formation of submicron particles formed, apparently, by the products of biodegradation of the polysaccharide. These changes help to
reduce the morbidity of the developed wound dressings, as shown in in vivo experiment.

References
Results from any computer simulation tool cannot be any better than the nuclear cross section data it uses. Cross section data are available to the users, in the form of evaluated data libraries like ENDF/B, JEFF, JENDL, etc. In these evaluated data libraries, the energy range of the neutron interaction varies from few electron-volts (meV range) to higher energies (~20 MeV). The neutron interaction data in the evaluated data libraries can be split into four major regions: thermal, resolved, unresolved and high energy regions. This postdoctoral assignment mainly deals with neutron interaction at low energies, i.e., thermal energy region. There is indeed a significant role of thermal neutron scattering cross section data in a wide variety of applications. The thermal data are needed for neutronics core calculations and benchmarks assemblies. Low-temperature thermal scattering data can also determine the effect of the crystal lattice and improve the knowledge of the resonance parameters. Such data are essential for cold moderator applications. Thermal scattering data for organic compounds are needed for neutron dosimetry and medical applications. Although a lot of progress has been achieved in improving nuclear data evaluation for fission, capture, and elastic cross sections, few progress has been done for double-differential scattering cross section and thermal scattering law for moderator materials.

In the standard scattering cross section data libraries, the cross sections in the thermal energy range are described by a $S(\alpha, \beta)$ function which is often termed as $\alpha \beta$ thermal scattering law (TSL). Until recently, standard TSL data libraries have relied mostly on experimental data measured in the 60s and are based on physics models and approximations embedded in the LEAPR module of the NJOY code. During the past few years, there has been a renewed interest in reviewing these models and in generating new thermal scattering
libraries based on the recent advancement in the time-of-flight (TOF) experiments and improved computational capabilities. Several groups have proposed different methodologies to produce TSL for different moderators. A promising technique providing reliable TSL involves Molecular Dynamic (MD) simulations. This method allows the computation of TSL directly using classical MD trajectories but is not completely model-free, due to the intrinsic limits of applicability of the used force-fields. Other techniques rely on a combination of MD with available experimental data to calculate the parameters of thermal scattering models like the one implemented in the LEAPR module of the NJOY code.

There is a need for reviewing existing thermal scattering data evaluations and developing new processing methodologies to improve and expand their applicability. Using better physics models, interpretation of TOF experimental data and MD simulations, the accuracy and reliability of the existing cross section data can be improved and the uncertainties in the cross sections can be quantified. The postdoctoral work at CEA is to revisit the limitations of the LEAPR module of the NJOY code and develop a new data processing tool (module) within the framework of nuclear data processing code GALILÉE-1 under development at CEA-Saclay. It is envisioned that this postdoctoral assignment will provide the opportunity to explore mechanisms to address issues regarding TSL determination at any temperature within a reasonable amount of time for Monte Carlo applications (for example, Doppler on-the-fly). The verification and validation of the developed methodology will be carried out using existing reactor and criticality safety benchmarks. Also, the developed methodology will be implemented into Monte Carlo codes to generate TSL on the fly within the Monte Carlo environment. The viability of the approach for generating TSL on the fly will be thoroughly examined so as to ensure its practicality.
The contact angle measurement on a porous montmorillonite clay before and after its sulfuric acid treatment

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The main aim of this study is determining the change in wettability of the Prrenjas clay of the montmorillonite type, after its sulfuric acid activation by determining the contact angle of clays with water. Prrenjas clay samples were activated with three different H2SO4 concentration 184 %, 491 % and 1113 % calculated against the clay dry mass. The contact angles between clay samples and water were determined by Thin Layer Adhesive Tape Wicking (TLATW) technique using methanol as total spreading liquid. Washburn equation is used to calculate the contact angle out of the rate of wicking on the adhesive tape. The Differential Light Scattering (DLS) technique was used to determine the particle size distribution of clay samples. The most present particle size results to be similar with the effective radiiuses calculated using the methanol wicking rate in the Washburn equation, around 170 nm for the untreated Prrenjas clay and 240 nm for the Prrenjas clay treated with 1113 % sulfuric acid. Fourier Transformed Infrared Spectroscopy (FTIR), used to determine the chemical changes after the acid treatment of the Prrenjas clay shows that the hydroxyl groups bounded in the clay metals Fe, Al and Mg almost disappears. It leads to a hydrophobization of the clay surface since its water contact angle changes from 70° for the untreated clay to similar values of 84° for the clays treated with 184 %, 491 % and 1113 % H2SO4.

Keywords: acid activation, contact angle, surface energy
Nitrogen-doped carbon nanotubes with different diameters and their nanocomposites with NiO as efficient electrocatalysts for hydrogen evolution reaction

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Multi-walled carbon nanotubes (MWCNTs) have superior properties as a good electricity conductivity, the high surface area, a resistance to strong acids and bases, incredible mechanical flexibility and strength. Doping MWCNTs with nitrogen heteroatoms donate of additional electrons to the delocalized $\pi$ system of the hexagonal carbon framework and enhance their electric conductivity. Incorporation of the nitrogen atoms in the structure of the carbon nanotube can also create defects in the tube walls that can act as active centers [1].

Hydrogen is considered as alternative for replacing fossil fuels due to its environmental friendly, purity and high energy density. The production of hydrogen by water splitting is a key component of clean-energy technologies [2]. Pt is the greatest known catalytic material for cathode water reduction in the hydrogen evolution reaction (HER, $4\text{H}_2\text{O} + 4e^{-} \rightarrow 4\text{OH}^{-} + 2\text{H}_2$) due to low overpotential in comparison with other electrocatalysts. However, Pt is expensive and source limited that significantly hamper their widespread applications. Some potential candidates for this process are catalysts based on compounds of transition metals such as Ni in alkaline media. However, metals and metal compounds have poor adhesion to the surface of the electrode. Therefore, nitrogen doped multi-walled carbon nanotubes (N-MWCNTs) have recently gained more attention as catalyst and as catalyst support for the HER.

Thus, the aim of this work was to study the effect of structure (diameters) of N-MWCNTs obtained by catalytic CVD method from acetonitrile and structure of their nanocomposites with NiO on their activity in electrocatalytic hydrogen evolution reaction in alkaline
media. N-MWCNTs were obtained on the co-precipitated catalysts based on Ni active phase and different supports (MgO and CaO) by the thermal decomposition of acetonitrile at 700 °C (CVD method) with subsequent purification of them in diluted HNO₃. For the preparing of the NiO/N-MWCNTs composites the purified samples of N-MWCNTs were sonicated in Ni(NO₃)₂·6H₂O water solution. The resulting colloid was filtered and dried and obtained powder was placed into the quartz reactor and was heated to 500 °C in Ar gas flow. After reaching the desired temperature these conditions was kept for 30 minutes. The structure of N-MWCNTs were characterized using transmission electron microscopy (TEM), high resolution transmission electron microscopy (HRTEM), scanning electron microscopy (SEM) X-ray Diffraction (XRD), infrared spectroscopy (IR) and X-ray photoelectron spectroscopy (XPS), CHN analysis and nitrogen adsorption-desorption method. The obtained materials were tested in the HER reaction. For this linear sweep voltammograms (LSV) were performed on a potentiostat Elins P8-S at room temperature, using a conventional three-electrode system equipped with a glassy carbon counter electrode, an Ag/AgCl reference electrode and working glassy carbon electrode (GC) (Metronm) that immersed in 0.1 KOH water solution.

Figure 1. TEM-images of N-MWCNTs-28 (a), N-MWCNTs-47 (b) and their outer diameters distribution respectively ((c), (d)) and polarization curves of
It was determined that the synthesized N-MWCNTs are significantly different in diameters and (Fig 1(a)-(d)). As can be seen from Fig. 1(e) the beginning of hydrogen reduction slightly shifted to less negative potentials in case of GC modified by N-MWCNTs-28 compare to electrode modified by N-MWCNTs-47. Thus, the GC electrode modified by N-MWCNTs with smaller diameters has higher electrocatalytic activity.

![Image](a)

![Image](b)

![Image](c)

![Image](d)

![Image](e)

Figure 2. TEM-images of NiO/N-MWCNTs-27 (a), NiO/N-MWCNTs-47 (b) and size distribution of NiO in these samples respectively ((c), (d)) and polarization curves of HER for GC electrode and GC modified by NiO/N-MWCNTs-28 and NiO/N-MWCNTs-47 (e).

The Figure 2a-b displays the TEM images of nanocomposites of obtained N-MWCNTs with NiO. It is seen that by use of the N-MWCNTs with bigger diameter (47 nm) result in the formation of the smaller NiO nanoparticles (with <d>=8 nm) while in nanocomposite with N-MWCNTs 25 nm the mean size of NiO nanoparticles is equal to 13 nm. From polarization curves presented in Fig 2 it can be seen that the NiO/N-MWCNTs-28 nm shows significantly higher electrocatalytic activity. Thus, it can be concluded that the increasing of the N-
MWCNTs diameters significantly effect on activity not only of undoped nanotubes but also of their nanocomposites with NiO.

References
New Rh(III) complexes forming ordered supramolecular aggregates in water

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Molecules that have the ability to self-assembly in water in supramolecular ordered phases are very interesting both for theoretical and practical point of view. The study and investigation of their self-assembling mechanism can bring important developments in comprehending the complex processes find in nature based on weak non-covalent intermolecular interactions. Many biological systems (liposomes, enzymes, cell membranes, DNA, myelin, viruses) exhibit liquid crystalline behavior, and in particular several drugs, dyes, nucleic acids and short chain DNA are chromonic in nature. Thus, the study of non-covalent interactions is crucial to understand many biological processes from nature that rely on these forces for structure and function.

Chromonic phases are considered a sub-class of lyotropic liquid crystals although they have distinct molecular features and liquid crystalline properties and structures. High coordination number complexes that self-assemble into chromonic or chromonic-like phases are intriguing because they do not apply to the basic molecular requirements of chromonics: planar cores (for self-assembly into columnar structures) and solubilising groups at the periphery.\cite{1,2} However, lately some tetrahedral Ag(I) and octahedral Ir(III) coordination complexes were reported to assemble in water into chromonic or chromonic-like phases.\cite{3-5} The classification of these complexes into the chromonics class or in a new class of materials is tricky, requiring the development of a library of such complexes and investigation of their self-assembling mechanism and liquid crystalline structures and properties.

On this background, the synthesis and characterization of new Rh(III) coordination complexes structurally analogues with the Ir(III) complexes previously reported was made. Their chemical structure is presented in Scheme 1.
The complexes exhibit self-assembling properties in water, as observed on POM, the textures observed being typically chromonic. The self-assembly of these complexes was investigated by SANS, NMR techniques and rheology. Moreover, in order to elucidate the nature of the Rh(III) complexes mesophase an investigation of the miscibility criterion with a well-known chromonic dye (Sunset Yellow FCF, known as “E110” in Europe) was carried out by POM and NMR. Further useful informations may be obtained by studying these mixtures by SANS.

References:
Enhancing transport properties of Bi-based HTS’s via doping with boron-containing dopants

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Superconductivity is one of the most important discoveries of the 20th century, which has a wide area of technological application. A phenomenon of superconducting materials resistance zeroing and ideal diamagnetism ability (Meissner Effect) expressed a perspective of energy lossless transportation and creation of high effective superconducting magnets.

Among superconducting materials, the bismuth-based (Bi,Pb)2Sr2Ca2Cu3Oy compound, called Bi(Pb)-2223, is the one of the most interesting for its great potential for large-scale applications in the no-loss electric power industry. After the discovery of Bi-based superconductor [1], tremendous efforts have been undertaken to accelerate the formation of (Bi,Pb)2Sr2Ca2Cu3Oy materials and improve their current carrying capacity. But after more than two decades, the formation of pure Bi(Pb)-2223 superconducting material having enhanced current carrying capacity (Jc) is still an open subject in the field of applied superconductivity.

A lot of promising results have been obtained in our lab during the last years in order to accelerate formation of (Bi,Pb)-2223 superconducting phase and improve critical current density by using the micro- and nanosized boron-containing dopants. Various dopants have been used — boron nitride-BN, boron carbide-B4C, strontium borate-Sr(BO2)2, lead borate Pb(BO2)2, boron oxide – B2O3, elementary boron – B [2-5].

XRD analyses results show that ~2-3-times acceleration of 2223 phase formation takes place. Beside this, we observe ~1,5-times increase of Jc of doped samples in case of microsized dopants in comparison with undoped (reference) (Bi,Pb)2Sr2Ca2Cu3Oy specimen. Moreover, 2-3 times increase of critical current density takes place in case of high-energy ball milling of precursor powder.
Materials and methods: solid-state reaction method; multilevel thermal treatment; manual and high-energy ball milling (planetary mill Fritsch Pulverisette 7); pressing of pellets using thermally elaborated material; XRD phase analyses; Jc critical current measurements, SEM analyses.

Material outcomes: using various boron-containing dopants, the best powder samples with 2223 phase high level and high Jc are applied in the short-length (5-10 cm) experimental superconducting wires, which are being fabricated with the PIT (Powder in Tube) technology.

One more possible application: based on the obtained results, the best material will be tested in thin films, using laser deposition technology. This is a subject of my studies in the limit of short-time project, part of which will be implemented (in case of approval) in Thin Films Department, at MFA, Budapest, Hungary (http://www.thinfilms.hu). In case of project success, there will be necessary to use the Neutron Scattering and Reflection Technique for measuring the structure of thin films and studying their properties.

References:
High-entropy alloys, which consist of five or more alloying elements in equal molar ratios, are an intriguing new class of structural materials. Despite the complex chemistry, they can form a single phase solid-solution with an incredibly simple lattice. CrMnFeCoNi is a face-centered cubic (FCC), for example. Several deformation mechanisms are known to operate in high-entropy alloys. At room temperature, CrMnFeCoNi deforms like a conventional FCC alloy, showing clear stages of dislocation slip and dislocation entanglement. At liquid-nitrogen temperature, the dominant deformation mechanism changes from dislocation to twinning, leading to high strength and large ductility. Here we show that, at even lower temperature, the serrated deformation dominates. Deformation behavior of CrMnFeCoNi high-entropy alloy was studied at 15K by in-situ neutron diffraction, to obtain insights of the effect of low temperature on the underlying deformation mechanism and the corresponding evolution of structure. The in-situ neutron diffraction data thus obtained clearly revealed crossover of different mechanisms and their demarcation points with deformation. The ultra-high strength of ~2.5GPa was achieved for the single phase CrMnFeCoNi high-entropy alloy with enhanced ductility at 15K mediated by serrated deformation, thus overcoming the strength-ductility trade-off, and showing the potential of this alloy for structural applications at low temperatures.
Application of the Neutron Noise Technique in the RA-4 Nuclear Reactor

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The neutron noise concept can be explained analyzing the response of a system of neutron detection in a stationary reactor. Neutron noise is defined as the fluctuation of the neutron count rate from its mean value. These fluctuations are related to some characteristics of the multiplicative system, i.e. the reactor, and it is possible to obtain dynamic information of the system by measuring these fluctuations. In particular, the analogous methods of neutron noise, $\alpha$ -Rossi and $\alpha$ -Feynman allow to determine physics parameters of interest such as the prompt neutron decay constant $\alpha_p$. From it, the reactivity value of the reactor in subcritical state and with external neutron source can be obtained. This reactivity is one of the most important parameters of both nuclear reactor and of any set of fissile material which can eventually cause a criticality accident.

In the present work the $\alpha$ -Feynman method was applied to the research and training nuclear reactor RA- 4, of power 1 W, in subcritical state and with external neutron source. The prompt neutron decay constant $\alpha_p$ was obtained, as well as the reactivity values of the reactor for different positions of one of its control rods.

This allowed to obtain the reactivity value of the control rod, as well as, the prompt neutron decay constant in the critical state $\alpha_c$.

Keywords: neutron noise, $\alpha$ -Feynman, $\alpha$ -Rossi, reactivity, subcritical state.
Morphological and thermal investigation of alginate membranes doped with magnetic nanoparticles

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A series of sodium alginate membranes doped with CoFe₂O₄ nanoparticles and cross-linked with Ca²⁺ ions were prepared by solution casting. The membranes thus obtained were characterized by using Fourier transform infrared spectroscopy (FT-IR), thermogravimetric analysis (TGA) and scanning electron microscopy (SEM).

SEM studies indicate that the surface morphology of uncross-linked and cross-linked alginate membranes containing CoFe₂O₄ nanoparticles is influenced by the presence of Fe³⁺ and Co²⁺ cations in the formulation of the cross-linked membranes and they compete with the effect of Ca²⁺ cations on the alginate polymer [1]. From the FT-IR and TG analysis, we can observe that the addition of CoFe₂O₄ nanoparticles does not affect the structure of the sodium alginate. It only intensify some peaks in the IR spectra and from the TG curves we can observe that the presence of nanoparticles make the membranes more thermostable [2-4].

The complementary use of alginate and magnetic nanoparticles can lead to new biomedical and biotechnological applications, including targeted drug delivery, magnetic cell separation, enzyme immobilization, magnetic resonance imaging (MRI), and hyperthermia treatments.
References:

The influence of the content of the Triton X-100 on the size, aggregation number and shape of binary mixed micelle with different Polisorbate surfactants

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The excess Gibbs energy describes thermodynamic stabilisation of a real mixed micelle related to the ideal binary mixed micelle, and it is usually expressed with the regular solution theory as well as with the Margules function of the second order. For comparing applicability of these two models is suitable a binary mixture of surfactants in which one component is conformationally rigid hydrophobic segment (Triton X-100) and the other component has coformationaly flexible hydrogencarbon segment (Brij S10 (S20). Experimentally spectroflotofluorimetrically by the method of pyrene as a probe molecule were determined critical micellar concentrations of binary mixed micelles of Tritona X-100 and Brij S10 as well as Tritona X-100 with Brij S20, with different molar fractions of system components and on different temperatures and thermodynamic parameters characteristic for binary mixed micelles. Experimentally determined critical micelle concentrations for mono component and binary mixtures of surfactants increase with the rise of the temperature starting from 298,15K, which is in accordance with the general theory of self-determination. Critical micelle concentration of Brij S10 and Brij S20 surfactants is lower than the critical micelle concentration of Triton X-100 since Brij surfactants are more hydrophobic. The composition of examined binary mixed micelle depends on the applied method. The size, shape and aggregation number of these aggregates should be confirmed by the small angle neutron scattering and we wish to study how temperature influences these parameters. Rodenas method suggest great polidispersity of micellar particles related to the regular solution theory, and both applied model suggest to synergistic interactions between building units in a binary mixed micelles Brij S10 (S20) – Triton X 100.
Controlling magnetic contrast in manganite superlattices

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The hole doped manganites have various electric and magnetic ground state, and these states can be controlled by hole doping ratio. In our previous report, we attempted cation ratio control of Nd$_{1-x}$Sr$_x$MnO$_3$ (NSMO) during deposition by control of oxygen pressure, and we grew two kinds of NSMO thin films with different hole doping (Nd$_{0.7}$Sr$_{0.3}$MnO$_3$ and Nd$_{0.5}$Sr$_{0.5}$MnO$_3$). These NSMO films show similar structural properties due to similar electron scattering length densities, but different magnetic properties. In this work, we grew superlattice by stacking NSMO with differently hole-doped NSMO (Nd$_{0.7}$Sr$_{0.3}$MnO$_3$ and Nd$_{0.5}$Sr$_{0.5}$MnO$_3$) as sublayers. The x-ray diffraction shows our NSMO superlattice has flat interface. However, there is no evidence on the formation of superlattices, because of their similar electron scattering length density. In addition, magnetic property of the superlattices shows enhancement of saturation magnetic moments compared to single layered NSMO films. This enhancement cannot be explained without magnetic interaction between sublayers. The polarized neutron reflectivity experiments showed existence of superlattice structure and magnetic interaction between sublayers in our superlattice NSMO film.

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Study on the photocatalytic behavior of \( \text{Cd}_{0.5}\text{Zn}_{0.5}\text{S} \) materials in different thermal conditions

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Since the discovery of photocatalytic water splitting on TiO\(_2\) electrodes \([1]\), materials with similar properties were intensively studied \([2-4]\). Most promising semiconductors for this aim are metal sulphides, due to their narrow band gap and good visible light absorption \([4-5]\). CdZnS, which is widely used in water splitting processes, is prone to photocorrosion caused by fast recombination of photo-induced electron–hole pairs \([6]\). Therefore new improvements were taken, involving different Zn source \([7]\), addition of noble metals \([8]\) or by introducing organic stabilizers \([9]\). By controlling the synthesis process, more suitable photocatalysts can be obtained, which was the aim of the present study.

In this study hydrothermally obtained \( \text{Cd}_{0.5}\text{Zn}_{0.5}\text{S} \) photocatalytic materials were investigated at different synthesis temperature (100°C, 150°C, 200°C and 230°C) and duration process (6 h, 12 h, 24 h, 48 h and 72 h).

Calculated band gaps from the UV-Vis spectra predicted good photocatalytic activity, with values that correspond to those found in related water splitting studies \([10]\). Materials obtained at different temperatures showed close band gap values, while for the second category of materials, an increase of band gap values was observed with the increase of the hydrothermal treatment duration.

Morphological parameters calculated from adsorption-desorption isotherms showed the importance of specific area and pore size distribution during different temperature and duration treatment applied on the studied compounds, leading to better understanding of the photocatalytic behavior of the materials.

It should be noted, however, that materials with ordered porosity exhibited even better photocatalytic results, in comparison to the ones
with high surface area, which is the case of materials treated thermally at different periods.

References

Microstructure investigation of positive electrodes of Li-ion batteries by the method of small-angle neutron scattering

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Currently, lithium-ion batteries are the most commonly used chemical sources of current. When considering the evolution of modern electronic devices, there is a clear tendency towards their miniaturization and increased functionality. This leads to a significant increase in energy consumption, which, in turn, requires the creation of more efficient and compact sources (accumulators) of energy. The work is aimed at conducting systematic studies of qualitative and quantitative patterns between the microstructure of electrode coatings and their specific characteristics. Information on the microstructure at all stages of the synthesis and modification of coatings will be obtained using small-angle neutron scattering, which, thanks to the high penetrating power of this radiation, allows us to study industrial systems within nondestructive testing.

The main goal of the work is to develop common practical criteria for optimizing the microstructure of the electrodes based on a wide range of active materials, nanostructured carbon additives and modified polymeric binders, which make it possible to achieve a significant gain in specific energy and power of lithium-ion batteries. Developed in the course of the project, scientific and technological solutions for the formation of electrode coatings with a given microstructure can form the basis for prototyping and creating domestic electrochemical energy storage devices with enhanced specific characteristics.
Structural analysis of aluminum oxohydroxide aerogel

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The oxidation of metallic aluminum through the amalgam layer upon exposure to humid air has been known for over a century [1]. Brittle amorphous aluminas which form during such an oxidation consist of fibres having a nanometric diameter. Optimization of the process (air humidity, temperature, addition of chemical modifiers etc.) allows obtaining large size alumina monoliths (several centimeters and even higher). The water content in such materials is close to 40%, their bulk density being only 13 kg m$^{-3}$ [2], thus they could be considered as alumina oxyhydroxide aerogels. However, the structure of these materials in mesoscopic range is still virtually unstudied. Such data are of primary importance to understand the mechanism of fibrous alumina monoliths formation.

The work presents the results of the comprehensive studies of the micro-and mesostructure of aluminum oxohydroxide aerogels, special attention was paid to the structural changes in these materials upon thermal annealing. Structural characterization of as-prepared and annealed aerogels was performed by means of complementary methods including X-ray diffraction, nitrogen adsorption-desorption, transmission electron microscopy, thermal analysis. Important structural information was
obtained using small-angle scattering techniques (SAXS, SANS and USANS).

It was found that the structure of aluminum oxohydroxide monoliths can be described within the three-level model: the primary particles (typical size of $r_c \approx 9–19 \, \text{Å}$) form the fibrils (cross-sectional radius $R \approx 36–43 \, \text{Å}$ and length $L \approx 3200–3300 \, \text{Å}$) or lamellae (thickness $T \approx 110 \, \text{Å}$ and width $W \approx 3050 \, \text{Å}$) which in turn are aggregated in large-scale structures (typical size $R_c \approx 1.25–1.4 \, \mu\text{m}$) with an almost smooth surface. High specific surface area of as-prepared aerogels ($\sim 200 \, \text{m}^2/\text{g}$) remains nearly unchanged upon thermal treatment up to $900^\circ\text{C}$. Sintering of alumina particles at higher temperatures ($1150^\circ\text{C}$) results in decrease of specific surface area down to $\sim 100 \, \text{m}^2/\text{g}$.

References
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<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jona Keri</td>
<td>Faculty of Natural Science, University of Tirana, Albania</td>
<td>22</td>
</tr>
<tr>
<td>Nataliia Lemesh</td>
<td>L.V. Pisarzhevskii Institute of Physical Chemistry, National Academy of Sciences of Ukraine</td>
<td>23</td>
</tr>
<tr>
<td>Emanuela Lombardo</td>
<td>University of Calabria, Italy</td>
<td>27</td>
</tr>
<tr>
<td>Giorgi Mumladze</td>
<td>Vladimer Chavchanidze Institute of Cybernetics of the Georgian Technical University</td>
<td>29</td>
</tr>
<tr>
<td>Muhammad Naeem</td>
<td>City University of Hong Kong</td>
<td>31</td>
</tr>
<tr>
<td>José Andrés Orso</td>
<td>National Atomic Energy Commission of Argentine (CNEA)</td>
<td>32</td>
</tr>
<tr>
<td>Alexandru Pahomi</td>
<td>West University of Timișoara, Romania</td>
<td>33</td>
</tr>
<tr>
<td>Ana Pilipović</td>
<td>University of Novi Sad, Serbia</td>
<td>35</td>
</tr>
<tr>
<td>Laura Riva</td>
<td>Polytechnic University of Milan, Italy</td>
<td>12</td>
</tr>
<tr>
<td>Sangkyun Ryu</td>
<td>Pusan National University, Korea</td>
<td>36</td>
</tr>
<tr>
<td>Paula Svera</td>
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<td>37</td>
</tr>
<tr>
<td>Meir Yerdauletov</td>
<td>Joint Institute for Nuclear Research, Dubna, Russia</td>
<td>39</td>
</tr>
<tr>
<td>Khursand Yorov</td>
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<td>40</td>
</tr>
</tbody>
</table>

43