

Poster Sessions

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The two compounds mentioned in the title ($\text{In}_{1.0}\text{Fe}_{0.1}\text{Te}_{0.9}$, $\text{In}_{1.0}\text{Co}_{0.1}\text{Te}_{0.9}$) are semimagnetic semiconducting materials of very useful application. The two compounds were prepared under Vacuum. X-ray diffraction patterns of the two compounds showed the presence of the same two different phases in each sample, one of the phases is InTe and the other is In_4Te_3 . No trace of Fe or Co was found in both samples or even as remains in the corresponding diffraction pattern. The quantitative phase analysis showed that InTe phase was a major phase of nearly 80% in both samples. Rietveld analysis were used in order to find the exact location of the Fe and Co atoms in the two phases in both samples, the In and the Te atoms positions were also found. The R factor of the refinement was found to be 0.09. The magnetization curve seems to show a paramagnetic properties for the two samples since the magnetic curves for the two samples pass through the origin. The saturation Flux were found to be 0.04545, 5.117, 2.689 emu/g for the pure InTe sample, the iron and cobalt Sample respectively. The MUD program were used in order to find the Crystallite size and microstrain in both phases for the two samples. The structural, microstructural properties of the two samples were correlated with each other

Keywords: semimagnetic semiconductor, structural analysis, crystallite size, microstrain

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Properties and local structure analysis of N or Nb doped TiO_2

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Until now, many kinds of photocatalysts have been developed, and particularly TiO_2 has been considered most promising for the strong oxidization ability. TiO_2 is one of most promising photocatalyst because of its optical and electronic properties, stability, low cost and non-toxicity. However, the excitation of pure TiO_2 by just ultraviolet irradiation has limited realization of effective utilization of solar energy because of 3-4% UV light in solar irradiation. In previous works reported that nitrogen doping could narrow the band gap and hence induce the visible light absorption of TiO_2 . On the other hand, transparent conducting oxides (TCOs) are key components in many optoelectric devices. Nb doped TiO_2 is a promising indium-free TCO. The purpose of this study is to examine the correlation between the band gap and the crystal local structure determined by Extended X-ray Absorption Fine Structure (EXAFS) analysis of N or Nb-doped TiO_2 . Results indicate that nitrogen doping could narrow the band gap and shorten the interatomic distances between Ti and O atoms in $\text{TiO}_2\text{:N}$. The reason for this is that in anatase-type structure $\text{TiO}_2\text{:N}$, O atoms approaches Ti atoms followed by the repulsive force operates between doped N atoms and O atoms. On the other hand, it was discovered that Ti-O interatomic distances in all samples of $\text{TiO}_2\text{:Nb}$, which were synthesized in different temperatures, were shorter than

Ti-O distance in non-doped TiO_2 . Moreover, it was found that the more the resistivity is low, the more Ti-O distance is long in the samples synthesized in different temperatures. These mean that the doping Nb atoms induces the enlargement of carrier concentration.

Keywords: photocatalysis, EXAFS, crystal structure and properties

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Crystal structural determination and SAXS/SANS structural analysis of human thrombomodulin domains

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Thrombomodulin (TM) is a membrane protein distributed in many different tissues with crucial functions in coagulation, fibrinolysis, cell proliferation, adhesion and inflammation. A unique feature of TM is regarding its intronless property. Current comprehension has been proposed to be a restriction in protein expression through regulation of different RNA splicing. Enhancement of blood coagulation function was not supposed to be through blood vessel per se, instead, possibly through pivotal mediations like thrombomodulin. The structures of TM are proposed to be responsible for its functions. The lectin-like domain of TM can be categorized as family containing C-type lectin, which is strongly involved in cell adhesion and inflammations, especially the properties regarding its carbohydrate recognition domain structure. As a consequence, it is absolutely essential to understand the structure of TM, in order to get into more functional details of its regulation in the aforementioned properties. Until present, there have been several NMR structures available for the TM fragments of EGF-4 and EGF-5 domains, Loop conformations as well as EGF-4,5 domain. Through X-ray crystallographic analysis, EGF-4 or EGF-5 fragments and complex structure of EGF-5 and thrombin have been also available. However, these so-far available structures, either through NMR or through X-ray analyses, can not shed light into the decent structural-functional interpretations for TM regulations in its crucial cellular functions. However, we have already got fairly abundant results in the crystallization of extracellular fragments of TM. Hopefully we will get into the structural and functional details of TM's molecular mechanism in the near future.

Keywords: thrombomodulin, X-ray crystallographic analysis, SAXS

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Structural and magnetic investigations of nanocrystalline nickel ferrite NiFe_2O_4

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Nickel ferrite is an important high frequency magnetic material due to its ultrahigh resistivity. Nanocrystals of NiFe₂O₄ ferrite have been synthesized by the chemical co-precipitation of the amorphous metal hydroxides (under controlled pH values). The prepared powders have been sintered at 800 C. Room temperature X-ray measurements of the prepared samples of NiFe₂O₄ reveal the production of single cubic phase with average crystallites size of about 30 nm, Results confirmed by transmission electron microscope (TEM) investigations. The lattice parameters, the oxygen position and the cation distribution have been determined by using Rietveld analysis. The study shows clearly surprising departure of the cation distribution from the known inverse distribution and reduce concentration of iron ions on tetrahedral sites, the degree of inversion is determined. The results of Mossbauer Effect spectroscopy (ME) and the Vibrating Sample Magnetometer (VSM) indicate the correlation between the magnetic properties and the nanocrystallinity of the investigated nickel ferrite.

Keywords: nanomagnetism, ferrites, magnetic - structure properties

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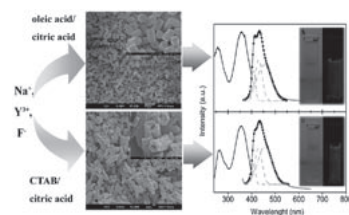
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Synthesis and intense blue luminescence of sodium yttrium fluoride microcrystals

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NaYF₄:Eu²⁺ microcrystals with an intense blue luminescence were fabricated. Oleic acid and cetyltrimethylammonium bromide were used as the surfactants to tune the morphology, while citric acid was taken as a ligand to stabilize the beta phase NaYF₄ and to reduce Eu³⁺ to Eu²⁺ for activation of blue luminescence. All as-prepared samples were found to crystallize in hexagonal rods or tubes. Both rods and tubes were capped with surfactants which enabled their stable dispersion in glycol to form transparent solutions. This observation seems to be the first example of the successful preparation of stable dispersion of micron luminescence solids. These transparent solutions showed an intense blue luminescent emission of Eu²⁺ with a quantum yield of about 14 percent. Finally, the mechanism for the fabrication of the rods and tubes as well as the reduction of Eu³⁺ ions was discussed.



Keywords: hydrothermal synthesis, inorganic luminescence, surfactants

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Solid-state optical properties of CT complexes with ammonium anthracene-2,6-disulfonate and TCNB

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The tuning of electronic properties by controlling the molecular arrangements in organic solid is an effective approach for both fundamental and practical research of the organic material. We have proposed that tunable solid-state optical properties of organic salts of anthracenedisulfonic(ADS) acid with aliphatic amines ascribed to arrangements of anthracene moieties. Recently we applied the tuning method to charge transfer (CT) complexes and founded that ammonium anthracene-2,6-disulfonate included 1,2,4,5-tetracyanobenzene(TCNB) to form CT complexes. Here we report several crystal structures and solid-state optical properties of the CT complexes composed of diisopropylamine, anthracene-2,6-disulfonate and TCNB. From crystallization under different conditions, we obtained three CT complex crystals, 1-3. X-ray structure analysis revealed that complex 2 and 3 have alternating stacks of 2,6ADS and TCNB molecules in which ratio are 1:1 and 1:2, respectively. On the other hand, Complex 1 has 1:1 segregated stacks. They showed very different solid-state optical properties depending on their different manners of molecular packing.

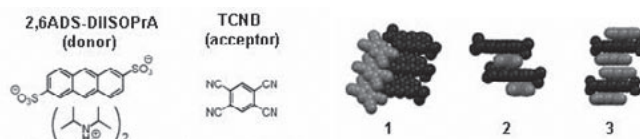


Fig.1 Molecular structure of donor and acceptor. Fig.2 crystal structure of complex 1,2 and 3.

Keywords: charge-transfer complexes, solid-state spectroscopy, single-crystal X-ray analysis

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Crystal and magnetic structure of quantum spin-trimer compounds Ca₃Cu_{3-x}Ni_x(PO₄)₄

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Ca₃Cu₃(PO₄)₄ is a novel quantum spin trimer system in which the three Cu²⁺ (S=1/2) spins are antiferromagnetically coupled giving rise to a doublet ground state (TN<1 K). By substituting a Cu²⁺ spin in the trimer by Ni²⁺ (S=1) a singlet ground state can eventually be realized offering for the first time the observation of the Bose-Einstein condensation (BEC) in a quantum spin trimer system. Neutron diffraction experiments with the powder samples of Ca₃Cu_{3-x}Ni_x(PO₄)₄ (x=1,2) have been carried out on HRPT and DMC instruments at SINQ to determine the arrangement of the Cu and Ni atoms in the trimers and to study possible magnetic ordering. The composition with one Ni per trimer (x=1) crystallizes in a monoclinic structure (sp. gr. P21/a, N14) with the cell parameters a=17.714 Å, b=4.885 Å, c=8.846 Å and β=123.845° at T=290K. Each trimer is formed by two crystallographic positions (2a) in the middle and (4e) at the ends of the trimer. We found that the middle position is occupied by the Cu²⁺, whereas the end positions are statistically equally populated with the Cu²⁺ and Ni²⁺. Thus, the three different types of trimers are present: Cu-Cu-Cu, Ni-Cu-Ni and Ni-Cu-Cu.