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Keywords: protein-ligand docking, DPI, drug discovery

MS95 ADVANCED FUNCTIONAL MATERIALS (INCLUDING MOLECULAR BIOLOGICAL FUEL CELL BATTERY)

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New Approach to Structure Determination of Crystalline Polymer Electrolytes

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Polymer electrolytes consist of salts, e.g. NaI, $\text{LiN}(\text{SO}_2\text{CF}_3)_2$, dissolved in high molecular weight polymers, e.g. poly(ethylene oxide) (PEO). The recent discovery of ionic conductivity in crystalline polymer electrolytes [1] was prompted by the elucidation of the crystal structure of $\text{PEO}_6\text{:LiAsF}_6$ [2] from powder diffraction data using a simulated annealing technique [3]. This challenged the established view that conduction occurs exclusively in amorphous polymer electrolytes above their glass transition temperature and opened a new avenue in polymer electrolyte research.

Recently we have established even more complex crystal structures of polymer electrolytes, such as $\text{PEO}_8\text{:NaBPh}_4$ and $\text{PEO}_4\text{:ZnCl}_2$, using a combination of single crystal diffraction data from a material prepared with a low-molecular weight polymer and powder data from a material with the same chemical composition but synthesized using a high molecular weight PEO. The combination proved to be successful when the individual methods failed to produce a reliable structural model.

We have also discovered polymorphism in $\text{PEO}_6\text{:LiAsF}_6$ and determined the crystal structure of the new phase. The differences in the crystal structure of the two polymorphs account for the difference in their ionic conductivity.

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Keywords: polymer electrolytes, ionic conductivity, polymorphism

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Magnetic Control of Electric Polarization in Magnetic Oxides with Non-collinear Magnetic Structures

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Recent observations of gigantic magnetoelectric and magnetocapacitive effects in rare-earth manganites, TbMnO_3 and DyMnO_3 [1,2], provide a novel approach to the mutual control of magnetization and electric polarization in magnetic ferroelectrics. We can control the magnitude and/or direction of the electric polarization vector by the application of magnetic field in these manganites. In comparing the results from the both manganites, we noticed that a characteristic common to the both materials is that they possess modulated magnetic structures with long wavelengths (as compared to the chemical unit cell) which arise from competing magnetic interactions. Ferroelectricity in these materials appears to originate from the competing magnetic interactions which cause lattice modulations through magnetoelastic coupling. In this talk, we show magnetic control of electric polarization in several magnetic oxides with non-collinear magnetic structures, which may provide new route to design magnetoelectrics.

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Keywords: multiferroics, magnetoelectric effect, non-collinear magnetic structure

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Crystal Structure and Magneto-transport Properties of New Cobalt Based Layered Oxides

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The search for new layered cobalt based oxides is very important to discover interesting physical properties as recently illustrated by the discovery of a large thermoelectric power in the metallic phase $\text{Na}_{0.5}\text{CoO}_2$ [1] and by the report on the superconductivity of the derived hydrated compound $\text{Na}_{0.3}\text{CoO}_2 \cdot 1.3\text{H}_2\text{O}$ [2]. Recent investigations in the Sr-Co-M-O systems (M = Ga, Ti...) by means of transmission electron microscopy techniques have allowed to detect new layered cobaltites. Their structure has been obtained by combining high resolution images and powder X-ray/neutron diffraction data.

Firstly, a new oxide, $(\text{Ga}_{1/3}\text{Co}_{2/3})_2\text{Sr}_2\text{CoO}_{6+\delta}$, has been isolated [3]. Its complex structure is described from a modulation vector $q^* = q_1a^* + q_2c^*$. For the as-prepared sample ($\delta \approx 0.4$), it can be described in an orthorhombic supercell $Bb2b$ ($q_1=1/3$ and $q_2=1$) with the unit cell parameters $a=3a_p\sqrt{2}$, $b=a_p\sqrt{2}$ and $c=19.2034(4)$ Å. The layer stacking consists in an intergrowth between a $[\text{SrCoO}_3]$ perovskite-type block and a block of triple $[\text{AO}]$ layers, $[(\text{SrO})(\text{Co}_{2/3}\text{Ga}_{1/3}\text{O}_{1+\delta/2})(\text{Co}_{2/3}\text{Ga}_{1/3}\text{O}_{1+\delta/2})]$ in which several kinds of GaO_x and CoO_x polyhedra coexist. Low resistivities ($\rho_{300\text{K}} \approx 10^{-1}\Omega\cdot\text{cm}$) depending on the δ value have been measured whereas a positive thermoelectric power $S_{300\text{K}} = 30\mu\text{V/K}$ indicates the presence of holes (Co^{4+}) in the CoO_2 conducting layers. This value can be compared with those observed in the $\text{Na}_{0.5}\text{CoO}_2$ and the misfit $[(\text{A}'_{1-x}\text{Co}_y)_{n-2}\text{A}_{2+x-y}\text{O}_n]^{\text{RS}}[\text{CoO}_2]_{b1/b2}$ ($\text{A}'=\text{Bi, Tl}$.. and $\text{A}=\text{Ca, Sr}$..) related cobaltites. Secondly, two hydrated oxyhydroxides have been prepared in air [4]. The structural study coupled to thermal analyses has shown that $\text{Sr}_3\text{Co}_{1.7}\text{Ti}_{0.3}\text{O}_5(\text{OH})_2 \cdot x\text{H}_2\text{O}$ and $\text{Sr}_4\text{Co}_{1.6}\text{Ti}_{1.4}\text{O}_8(\text{OH})_2 \cdot x\text{H}_2\text{O}$ are derived from the Ruddlesden-Popper $n = 2$ and $n = 3$ members, respectively. The T-dependence of the structure shows upon warming two broad structural transitions from hydrated oxyhydroxides to oxygen deficient RP structures via an anhydrous oxyhydroxide form. The phenomenon of water loss during warming up to 1000°C to obtain the parent RP structures is found to be reversible. The magnetic behavior of these phases is governed by the substituted amount of Ti^{4+} (d^0) for cobalt species : cluster-glass and spin-glass like properties are observed for the hydrated $n = 2$ and $n = 3$ members, respectively.

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Single-component Molecular Conductor Formed by Electron Transfer between d and π Orbitals

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Recently, research on conducting systems that consist of a single-component molecule has attracted a lot of attention.[1] Herein, we report the crystal structure and electronic properties of novel linear chain rhodium(I,II) mixed-valence complex, $\{\text{Rh}(3,6\text{-DBDiox-4,5-Cl}_2)(\text{CO})_2\}_\infty$ (**1**) where 3,6-DBDiox-4,5-Cl₂ is used to indicate the semiquinonate or catecholate form of 3,6-di-*tert*-butyl-4,5-dichloro-