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Keywords: protein tyrosine phosphatase families, MAP kinase families, focused structural proteomics

MS.85.5*Acta Cryst.* (2008). A64, C144**Focused structural proteomics of protein synthesis systems**

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Protein synthesis is performed by a large number of proteins and RNAs. We have been doing structural proteomics focused on protein synthesis in bacteria, archaea, and eukarya. The crystal structures of tRNAs, aminoacyl-tRNA synthetases, translation factors, and the ribosomal subunits will be discussed to describe the process of protein synthesis.

Keywords: protein synthesis, tRNA, ribosome

MS.86.1*Acta Cryst.* (2008). A64, C144**Complex perovskites: Chemical order, crystallographic distortions and physical properties**Patrick M Woodward¹, Graham M King¹, Rebecca A Ricciardo¹, Susana Garcia-Martin²

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This contribution surveys our studies of complex perovskites with a particular emphasis on atomic ordering over various length scales and its impact on the structural distortions and physical properties of these materials. I will show some examples of perovskites where cation ordering is critical for properties and applications. In the A_2MnMO_6 systems the coupling between orbital ordering (cooperative Jahn-Teller distortions) and octahedral tilting is demonstrated and exploited to control the magnetic properties of double perovskites. Next I will discuss $ALnMM'O_6$ ($A = Li^+, Na^+, K^+$, $Ln =$ rare-earth cation) perovskites where strong coupling between A-site ordering, B-site ordering and second order Jahn-Teller distortions of the B-site cations are all closely linked. Some of these materials show a fascinating periodic phase separation. They also exhibit coupling between magnetic ordering of transition metal and lanthanide ions that is promising for multiferroic behavior. Finally time permitting I will discuss our studies of oxynitride perovskites, AMO_2N ($A = Ba, Sr, Ca$; $M = Ta, Nb$), where novel dielectric behavior (high, nearly temperature independent permittivity) is closely linked to the details of the anion order.

Keywords: perovskites, magnetic oxides, oxynitrides

MS.86.2*Acta Cryst.* (2008). A64, C144**Local and long-range structure in LLTO perovskites with Li^+ superionic mobility**

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LLTO ($Li_xLa_{2/3-x/3}TiO_3$) is an excellent Li^+ ion conductor at room temperature ($10^{-3} S cm^{-1}$ for $x=0.3$), of interest as solid electrolyte in electrochemical devices. Structural studies by neutron powder diffraction showed perovskite superstructures with $2^{1/2}a_p \times 2^{1/2}a_p \times 2a_p$ tetragonal ($x>0.24$) and $2a_p \times 2a_p \times 2a_p$ orthorhombic ($x<0.24$) unit-cells, and $P4/nbm$ and $Cmmm$ symmetries. A partial La-Li ordering according to (001) layers is coupled to anti-phase octahedral tilts $a^0a^0c^0$ and $a^0b^0c^0$ for the tetragonal and orthorhombic cases. Li is heavily disordered within the A-type cage, accounting for the high ionic mobility. The local Li environment was studied by ab initio periodic quantum-mechanical simulations of selected ordered structural models. The phases $Li_{1/8}La_{5/8}TiO_3$ ($2a_p \times 2a_p \times 2a_p$, $Z=8$) and $Li_{5/16}La_{9/16}TiO_3$ ($2a_p \times 2a_p \times 4a_p$, $Z=16$) were considered, with Pm or PI symmetry, to represent the Li-poor and Li-rich compositions. Several different La-Li-vacancy ordering patterns within the (001) layers of A cages were devised. The structures were optimized by energy minimization, so as to localize the preferred lithium sites for each ordering scheme. It was found that the Rietveld-refined most populated Li site, close to the O_4 windows separating adjacent A cavities in the layer, corresponds to La-poor local configurations, and is actively involved in the ion migration process. The second populated site is related to La-rich local environments, and is a trapping location less favourable to ionic transport. By combining NPD results (long-range Li disorder) and ab initio simulations (local Li order), one- and two-dimensional atomistic pathways are proposed for Li^+ ion diffusion within the perovskite framework, including the prediction of activation energy barriers for ionic hopping.

Keywords: solid electrolytes, *ab-initio* calculations, neutron powder diffraction

MS.86.3*Acta Cryst.* (2008). A64, C144-145**Size and strain effects in nanostructured relaxor and morphotropic compounds**Jean-Michel Kiat^{1,2}

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The field of morphotropic systems with giant dielectric and piezoelectric properties is very active, and many interesting results have been obtained, in particular in lead based-systems. However up to now, only very few papers have addressed the question of grain size reduction and its effect on the physical and structural properties of these materials. We will report results obtained in nanocrystalline powders and ceramics with controlled grain size from 15nm up to micrometric sizes, as well in thin films with several thicknesses from 40nm and different substrates, in $PbMg_{1/3}Nb_{2/3}O_3$ - $PbTiO_3$, $PbSc_{1/2}Nb_{1/2}O_3$ - $PbTiO_3$, and $BiScO_3$ - $PbTiO_3$ systems. The consequences on the dielectric properties and on the rotation of polarisation will be discussed and compared with the situation in bulk materials. In particular it will be shown that changing the grain sizes provides an easy way to tailor the direction of the polarization