resulting in ferroelectricity in $BiFeO_3$ is driven by a lone pair of the Bi^{3+} cation [2,3]. Due to similarity between the electronic structures of Bi^{3+} and Pb^{2+}, the substitution of Pb for Bi provides a potential way to modify the electric and magnetic properties of the mixed lead-bismuth ferrites.

Anion-deficient perovskites $(Pb,Bi)_{1-x}Fe_{1+x}O_{3-y}$ were prepared as single phases in the compositional range from $Pb_{0.857}Bi_{0.094}Fe_{1.049}O_{2.572}$ to $Pb_{0.409}Bi_{0.567}Fe_{1.025}O_{2.796}$. Variation of the anion content in the compounds is carried out through a long-range-ordered arrangement of crystallographic shear (CS) planes, which incommensurately modulate the basic perovskite structure. Using a combination of electron diffraction and high-resolution scanning transmission electron microscopy, a superspace model was constructed describing a periodic arrangement of the CS planes of any possible orientations. The model was verified by refinement of the $Pb_{0.650}Bi_{0.308}Fe_{1.042}O_{2.675}$ crystal structure from neutron powder diffraction data ((3+1)D S.G. $X2/m(\alpha 0\gamma)$, $X = [1/2,1/2,1/2,1/2]$, $a = 3.8999(2)$Å, $b = 3.8924(2)$Å, $c = 4.0897(2)$Å, $\beta = 91.947(3)°$, $q = 0.05011(7)a^* + 0.09188(6)c^*$ at $T = 550$K, $R_P = 0.043$, $R_{wP} = 0.056$). The $(Pb,Bi)_{1-x}Fe_{1+x}O_{3-y}$ structures consist of perovskite blocks separated by CS planes confined to nearly the $(509)_p$ perovskite plane. Along the CS planes, the perovskite blocks are shifted with respect to each other over the $1/2[110]_p$ vector that transforms the corner-sharing connectivity of the FeO_6 octahedra in the perovskite framework to an edge-sharing connectivity of the FeO_5 pyramids at the CS plane, thus reducing the oxygen content. Variation of the chemical composition in the $(Pb,Bi)_{1-x}Fe_{1+x}O_{3-y}$ series occurs mainly due to a changing thickness of the perovskite block between the interfaces. The Pb, Bi, and Fe atoms are subjected to strong displacements occurring in antiparallel directions on both sides of the perovskite blocks, resulting in an antiferroelectric-type structure. This is corroborated by the temperature-, frequency-, and field-dependent complex permittivity measurements. $Pb_{0.650}Bi_{0.308}Fe_{1.042}O_{2.675}$ demonstrates a remarkably high resistivity > 0.1 TΩcm at room temperature and orders antiferromagnetically below $T_N = 608(10)$K.

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Protein Data Bank on the Semantic Web

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The Protein Data Bank (PDB) provides a wealth of structural information on biological macromolecules. However, modern biomedical research demands integrative approaches to elucidate the complexity of living systems, which in turn requires gathering various kinds of information from a wide range of sources. In such a context, no single database, such as the PDB, is useful by itself. Given the ever increasing number of databases, and the ever increasing amount of data made available in each of these databases, compiling all the databases into a single archive is not feasible, if not impossible. Therefore, an approach that allows distributed data resources to be integrated on demand seems more appropriate. The Semantic Web is one such framework.

In the Semantic Web, data are provided in the RDF (Resource Description Framework) format, possibly accompanied by an ontology specified in RDFS (RDF Schema) or OWL (Web Ontology Language). Ontologies allow Semantic Web agents to infer new information that is not explicitly stated in a database. In RDF, each datum is expressed as a triple of subject (URI for data resource), predicate (describing relations between two data), and object (URI or literal data).

In this poster, we present our attempt to convert PDB data into RDF with an OWL ontology converted from the PDB exchange dictionary. RDF files for all PDB entries were automatically generated from the corresponding PDBML files by using an XML style sheet, which was also automatically generated from the PDBML XML Schema by using another XML style sheet. An OWL ontology was generated from the PDBML XML Schema in a semi-automatic manner. Extensive cross-references are provided in RDF-formatted PDB entries, including those within each PDB entry, and between related PDB entries, and pointers to the PDB Chemical Component Dictionary, as well as pointers to external resources such as UniProt, PubMed, NCBI Taxonomy, and Bio2RDF. Each mmCIF category element in each PDB entry is given a dereferenceable URL so that agent programs can actually obtain the data on the Web by following the links. We discuss some technical issues concerning how to manage several billion triples in a daily basis in addition to some potential problems in the current PDB data encountered during the conversion from PDBML to RDF. The Web interface to PDB/RDF will be available at http://pdbj.org/rdf/

Keywords: database, web, computation

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Freezing of disordered hydrogen-bonding networks observed in nucleotide hydrates

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Nucleotides, basic components of nucleic acid, crystallize frequently in highly hydrated states. Layered structure is usually formed where an organic layer of nucleotides and an inorganic layer of water molecules and counter ions align alternately. Hydrogen bonds play a key role to construct layered structures in both organic and inorganic layers.

Disodium inosine 5'-monophosphate (Na_2IMP) and disodium uridine 5’-monophosphate (Na_2UMP) crystallize as octahydrate and heptahydrate, respectively. We have been examining humidity- and temperature-dependence of crystal structures by X-ray and neutron diffraction, gravimetric and thermal analyses. At room temperature, a considerable part of water molecules and counter ions disorder dynamically. The disordered sites are classified into several networks, and it indicates that disordered water molecules and sodium ions displace collectively switching their networks. With lowering temperature, the unit cell of each hydrate doubles and the disordered sites disappear at –150 °C. Freezing mechanism of hydration water will be discussed based on temperature dependence of interaction schemes.

Keywords: hydrogen bond, dynamic disorder, nucleotide

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Experimental Charge Density of Selected Amino Acids.

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According to reports [1], [2], a phase transitions in crystals of d-