

STRUCTURE DESIGN OF NEW PEROVSKITES

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Anion ordering in the perovskite structure (ABO_{3-x}) affects different physical properties. Thus, controlling amount of anions and their ordering in perovskites often means taking control over the desired electronic and/or magnetic properties. Various crystal chemistry factors influencing the anion sublattice will be discussed: the electronic shell structure of the B-cations, which determine oxidation states, coordination numbers and geometry of the polyhedra; mutual influence of the anion ordering and cation ordering at the A- and B-sublattice; the specific A-O coordination caused by the lone electron pair.

A combined influence of the lone pair of the Pb^{2+} cations and distorted octahedral environment of the V cations due to formation of short vanadyl bonds results in tetragonally distorted ($c/a=1.23$) $PbVO_3$ perovskite. Its crystal structure contains isolated layers of corner shared VO_5 pyramids in contrast to 3-dimensional octahedral network in cubic $SrVO_3$. A stereoactive lone $6s^2$ electron pair of Pb^{2+} cation plays also an important role in formation of crystallographic shear planes in the $Pb_{1-x}FeO_{3-y}$ structures. These CS planes consist of double chains of edge sharing distorted tetragonal FeO_5 pyramids, connected through FeO_6 octahedra by corner sharing. The building principle of these newly discovered CS structures in perovskites opens new opportunities for the design of novel perovskites as potential multiferroic materials.

Additional degree of freedom is provided by variation of the crystal chemical properties of cations in the A-sublattice. This approach has been applied for synthesis of Co-based perovskites. Ordering of two different A-cations (Sr^{2+} and R^{3+}) in Co-based anion-deficient perovskites results in formation of the $Sr_3RCo_4O_{10.5+\delta}$ structures. They can be described as alternating layers of corner-shared CoO_6 octahedra separated by layers consisted of tetra-cyclic units of CoO_4 tetrahedra. Variation of Co-valence by changing oxygen content strongly affects magnetic and conductivity properties of these perovskites.