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Oxide materials chemistry using single crystal and powder X-ray and neutron diffraction

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Mixed transition-metal oxides (MTMO) including stannate phases have promising material properties and are known for the ability to tailor particular features for different uses. They are currently being explored as possible alternative substrates in many emerging high-tech applications such as electrode materials in lithium-ion batteries and as conducting oxides in gas detector sensors [1-3]. The presentation will an overview about the preparation, crystallographic and characterization based on X-ray and neutron diffraction techniques of two groups of mixed transition metal-main group metal oxide materials and spinel compound. Layered oxide structures have been widely studied for their potential use in applications ranging from ferroelectricity to giant magnetoresistance in the field of semiconductor materials. The Fe based layered oxide Fe_{4-x}Mn_xSi₂Sn_yO₁₆ provides a novel situation in oxide compounds. It can be described as a composite of intermetallic (FeSn₆) clusters and (Fe/MnO₆)/(SnO₆) oxide layers within the one structure. SiO₄ tetrahedra separate these layers which leads to electronic and magnetic isolation of the repeated layers by about 7 Å resulting in a nearly perfectly 2D oxide system comparable to a one layer thick oxide "thin film". In this study, starting with Fe₄Si₂Sn_yO₁₆, we focus on analysing the electronic structure and its relationship to unique magnetic properties [4-5]. The presentation also summarizes the crystal and magnetic structures of novel iron and tin containing quaternary spinel structures (M_{2-x} Fex)SnO₄ (M =Mn, Zn and $0 \le x \le 2$). Neutron and synchrotron X-ray powder diffraction in combination with spectroscopic investigations (Mössbauer, IR and UV-Vis), magnetic measurements and SEM/EDX have been performed on the (M_{2-x} Fex)SnO₄ systems to find out the exact mechanism of Fe substitution, how much Fe and in what oxidation state is substitued and the effects upon the crystal and magnetic structure.



Biography

Tilo Söhnel did his PhD at the Technical University of Dresden, Germany, in the field of inorganic solid-state chemistry. After different post-doctoral positions in Germany and Auckland, he started as lecturer at the University of Auckland and is currently Associate Professor. His research interest lies in the field of experimental and theoretical chemistry of solid state compounds and inorganic materials such as mixed main group metal / transition metal cluster compounds and complex transition metal oxides. This includes the preparation and characterization of novel tin and antimony cluster compounds with promising materials properties and the calculation of band structures of solid-state compounds to investigate the crystal structure and the electronic structure. For the identification of these compounds the group intensively uses X-ray and neutron single crystal and powder diffraction techniques.

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