

coupled technique, PARallel Recording Of Dark-field Images (PARODI). It is a new breed of convergent beam electron diffraction developed at Brookhaven to accurately determine structure factors of low-order reflections that are sensitive to valence electron distribution. The synchrotron based single-crystal x-ray diffraction was used to determine the structure factors of high-order reflections that are sensitive to atomic positions and Debye-Waller factors. The two sets of experimental data were combined and refined, and then compared with DFT calculations. Examples on charge density studies including $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ oxide that exhibits extremely high dielectric constant (~ 104) over a wide range of frequencies and temperatures will be given [1,2]. Our recent work on electron scattering amplitudes involving non-spherical orbitals (p and d orbitals) of transition-metal elements will also be reported. We demonstrate that it is possible to accurately measure valence electron distribution, electron orbitals and bonding characteristics of complex functional materials using quantitative electron and x-ray diffraction. Collaborations with J.C. Zheng, L. Wu, J. Hanson, P. Northrup and W. Ku are acknowledged. This work is supported by U.S. DOE under Contract No. DE-AC02-76CH00016.

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Bonding electrons visualization in photo-excited state using synchrotron X-ray powder diffractometry

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The synchrotron X-ray powder diffractometry has been recognized as one of powerful methods for materials science research. By using Maximum Entropy Method (MEM) as an analytical method for the powder diffraction data, bonding electrons can be visualized to reveal the structure-property relationship. The reliability of the MEM charge density depends on 'accuracy' and 'precision' of experimental data. In present studies, we have succeeded in visualizing bonding electrons in the photo-excited state [1]. So far the accuracy of structural analysis under photo irradiation has not reached bonding electrons level. That can be attributed to inhomogeneous excitation caused by large difference between probe light (X-ray) and excitation light (visible laser) energy. In order to overcome the difficulties, we designed sample packing method into a capillary and photo irradiation system for homogeneous excitation. As a result charge density analysis under photo irradiation was successfully achieved in one of spin crossover complexes, $\text{Fe}(\text{phen})_2(\text{NCS})_2$, which shows a dynamical photo-induced phase transition (PIPT). The bonding nature between Fe and N under photo irradiation is clearly suppressed compared with both ground low-spin phase and temperature induced high-spin phase. The bonding nature created by visible laser may characterize the faster relaxation process of the dynamical PIPT. In my talk, charge density study of persistent PIPT materials (transition metal cyanides [2, 3]) and transient PIPT materials (charge transfer organic materials) will be presented with the dynamical PIPT material.

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Structure based design of new thermoelectric materials

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There is an urgent need to develop new environmentally friendly energy sources and improving energy efficiency in many technologies and processes. One interesting possibility is thermoelectric energy conversion. Thermoelectric materials are functional materials, which are attracting huge attention due to their dual ability of electrical-thermal energy conversion. Thus, thermoelectric materials are used either for cooling or for energy production. In spacecrafts the preferred method of energy generation is conversion of heat from a radioactive plutonium source to electricity using multi-step thermoelectric converters. There are a vast number of waste heat sources in modern societies that could be harvested in similar ways. In the talk the interplay between structure and thermoelectric properties will be discussed for a range of new complex thermoelectric materials. The materials design has particular focus on lowering the lattice contribution to the thermal conductivity e.g. by introduction of rattling guest atoms or interstitial atoms. The talk will cover materials with applications in high temperature (inorganic clathrates [1-3]) and intermediate temperature (zinc antimonides [4-6]) energy conversion as well as low temperature cooling (iron antimonides [7]).

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Experimental measurements of bond density at the Si(111)-7x7 surface

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Measurement of valance charge density, the distribution of electrons important to bonding, in bulk materials is a rather well established technique in the diffraction community. In principle, the ability to directly measure the charge density at a surface is at least as interesting as in the bulk, if not more so. The exact structure of these surfaces dictates their usefulness and, in particular, the charge density determines the physical, chemical, and electronic properties important to building a device, or designing a catalytic reaction. We have used a combination of electron and x-ray diffraction