Measurements of Valence Electron Distribution in Perovskite $CaCu_3Ti_4O_{12}$

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$CaCu_3Ti_4O_{12}$ oxide recently has attracted much attention due to its extremely high dielectric constant (~10^4) from static fields up to kilohertz frequencies over a wide temperature range (100~600 K) [1]. In this presentation we report our study of the electronic structure and charge distribution of the material by combined use of quantitative electron diffraction, x-ray diffraction and DFT calculations. The electron diffraction was based on our unique diffraction-imaging coupled technique [2]: PArallel Recording Of Dark-field Images (PARODI). It is a new breed of convergent beam electron diffraction developed 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 mainly used to determine the structure factors of high-order reflections that are sensitive to atomic positions and Debye-Waller factors. The experimental results were then compared with various DFT calculations. Our results show that quantitative electron diffraction now can be used to test DFT. Combing the three techniques we are able to reveal valence electron diffraction, electron orbitals and bonding characteristics of complex functional materials.

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[1] Subramanian, et al., *J. Sol. State Chem.*,2000, **151**, 323. [2] Wu L., et al., *Phys. Rev. B*, 2004, **69**, 064501.

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