Application of Synchrotron Charge Densities in Materials Chemistry

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The charge density (CD) of a molecular system is probably the most information-rich observable available to chemistry. It can be obtained either from quantum mechanical calculations or estimated experimentally from accurate X-ray diffraction data. The X-ray technique recently has been revitalized due to major advances in the experimental methods with the availability of area detectors, intense short wavelength synchrotron radiation and stable helium cooling devices [1]. This has produced significant improvements in data accuracy. We have for the last decade invested considerable efforts in measurement and interpretation of X-ray CDs of a wide range of systems such as metal organic framework system, thermoelectric materials, zeolites, molecular magnets, coordination complexes, oxidation catalysts, organic solids with strong hydrogen bonds and enzyme models. In this talk, recent materials chemistry applications of synchrotron based CDs will be discussed [2-7]

(1) P. Coppens et al., Coord Chem. Rev. 2004, 249, 179-195 (Charge density analysis using high-brightness synchrotron radiation)

(2) J. Overgaard et al. J. Am. Chem Soc. 2003, 125, 11088-11099 (The Electron Density Distributions of Redox Active Mixed Valence Carboxylate Bridged Trinuclear Iron Complexes)

(3) G. J. Snyder et al. Nature Materials 2004, 3, 458-463 (Disordered zinc in Zn4Sb3 with phonon glas, electron crystal thermoelectric properties)

(4) R. D. Poulsen et al., Acta Crystallogr. Sect. A. 2004, 60, 382-389 (Synchrotron charge densities in materials chemistry. 16 K X-ray charge density of a new magnetic metal-organic framework material, [Mn2(C8H4O4)2(C3H7NO)2])

(5) R. D. Poulsen et al., J. Am. Chem. Soc. 2005, 127, 9156-9166 (Synthesis, Physical Properties, Multi-Temperature Crystal Structure and 20 K Synchrotron X-ray Charge Density of a New Magnetic Metal Organic Framework Structure, Mn3(C8O4H4)3(C5H11ON)2)

(6) R. D. Poulsen et al., unpublished (Synchrotron X-ray charge density Study of Coordination Polymer Mn(HCOO)2(H2O)2)

(7) R. D. Poulsen et al., unpublished (Synchrotron X-ray Charge Density Study of an Unsymmetrical Linear Tricobalt Chain Complex, Co3(dipyridylamide)4Cl2 ?2.11CH2Cl2)