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Title: Ab-initio determination of X-ray structure factors of fcc-copper

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The static structure factors are very useful in analyzing the X-ray diffraction data, charge density, and thereby charge transfer and the bonding in solids. The structure factors are also derived from the ground state charge density distribution in solids. In this paper, we report the ground state property i.e. X-ray structure factors of fcc-copper. To compare the experimental data, the theoretical values are computed within the framework of linear combination of atomic orbitals (LCAO) method using Hartree-Fock (HF), density functional (DF) and hybrid B3PW schemes. Key Words: LCAO method, X-ray structure factors, 3d metal etc. *Corresponding author. Tel.: +91 1438-228648, Fax: +91 1438-228649 E-mail address: drpaalvi@gmail.com References [1] R. Dovesi, V.R. Saunders, C. Roetti, R. Orlando, C. M. Zicovich-Wilson, F. Pascale, B. Civalleri, K. Doll, N. M. Harrison, I. J. Bush, Ph. D'Arco and M. Llunell, CRYSTAL06 User's manual, University of Torino, Torino, 2006.