Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

First-principles study of x-ray linear dichroism at the Mn K edge of $LaMnO_3$ TATSUYA SHISHIDOU, TAMIO OGUCHI, ADSM, Hiroshima University — $LaMnO_3$ shows orbital ordering of Mn $3d$ ($3x^2 - r^2/3y^2 - r^2$) states associated with the cooperative Jahn-Teller distortion. Resonant x-ray scattering measured at the Mn K edge by Murakami *et al.* shows peculiar azimuth-angle dependence, indicating that the degeneracy of the Mn $4p$ states should be lifted. For its mechanism, two models have been proposed. One is the Coulomb mechanism, that is, the $3d$ orbital ordering causes the level splitting of the $4p$ states through the intra-atomic $3d$-$4p$ Coulomb interaction. The other is the Jahn-Teller mechanism: the $4p$ bands are strongly influenced by the Oxygen displacements, not by the anisotropic $3d$ charge distribution resulting from the orbital ordering. The important point to note is that these two models yield opposite way of the $4p$ splitting. To resolve this argument, very recently, Maruyama *et al.* have carried out x-ray photoabsorption measurements at the Mn K edge using linearly polarized light. The energy and polarization dependence of their spectra clear up the unoccupied Mn p states, apparently supporting the Jahn-Teller mechanism. Furthermore, they found interesting azimuth-angle dependence as a function of photon energy. For its interpretation, detailed band-structure information is undoubtedly necessary. In this talk, using the first-principles FLAPW calculations, we will discuss the overall feature of the measured spectra and its relation to the $3d$ orbital ordering and Jahn-Teller distortion.

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Date submitted: 30 Nov 2004 Electronic form version 1.4