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.