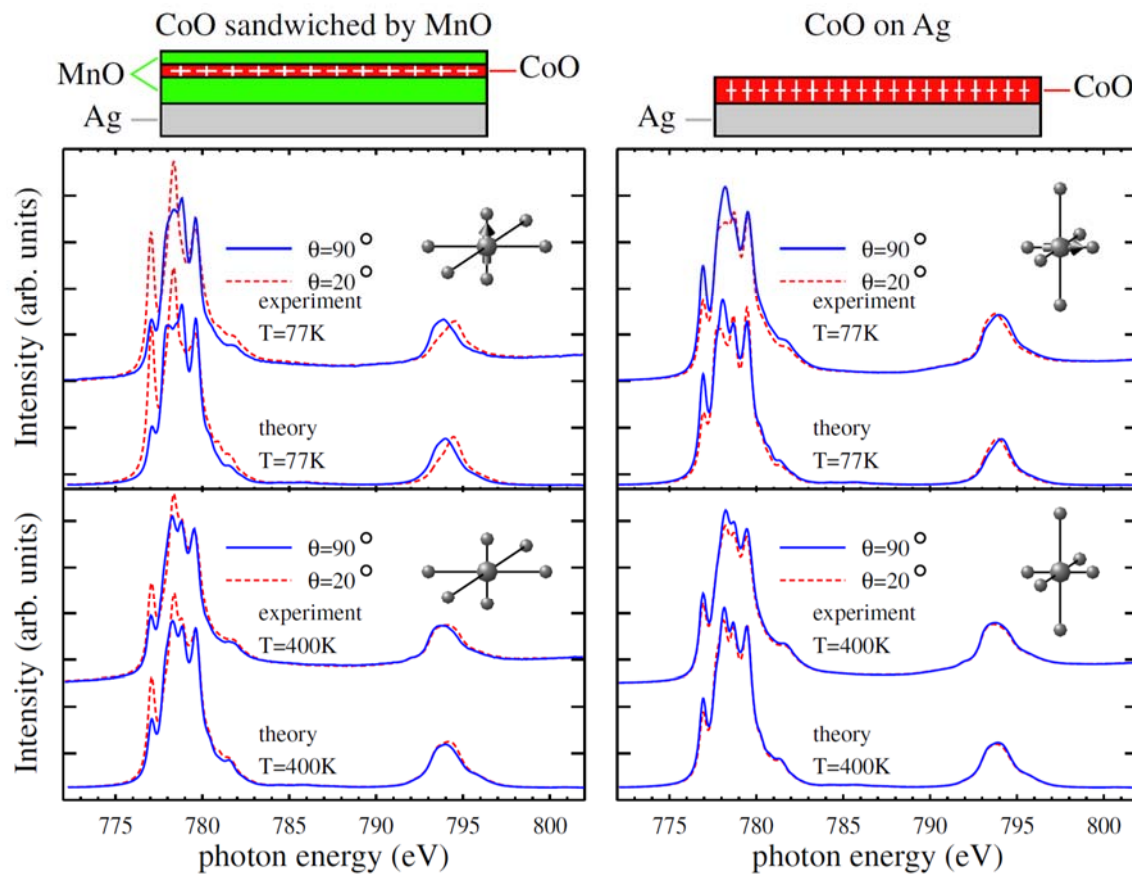


Linear dichroism of CoO in D4h symmetry



g) Calculate the 2p XAS spectrum of CoO on MnO and CoO on Ag. The symmetry is D4h; change the values of D_s from -40 to 40 meV in steps of 4, for $D_t = -12, -4, 4, 12$ meV. For which D_s and D_t values one obtains the better simulation? Use the following parameters in charge transfer calculations: $\Delta = 6.5$, $U_{dd} = 6.5$, $U_{pd} = 8.2$, $V_{eg} = 2.1$, $V_{t2g} = 1.1$, $10Dq(Ld) = 1.4$.