Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information.

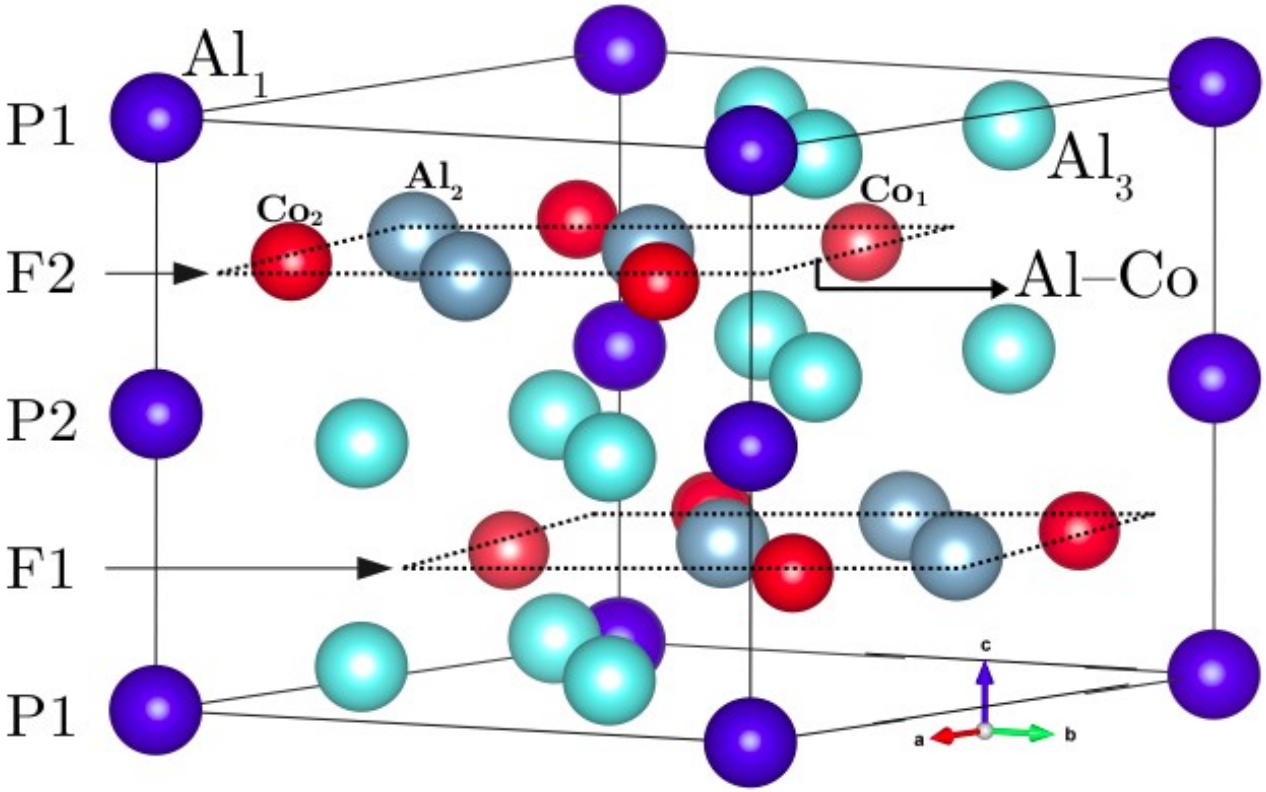

Figure 1: Hexagonal crystal structure of the compound Al_5Co_2 with blue atoms corresponding to Al and red ones to Co. The different shades of blue correspond to the different orders of Al by layer. We call Al–Co, the layer that contains the atoms Al_2, Co_1 and Co_2; We indicate the puckered layers (P) between the atoms of Al_1 and Al_3 and the flat layers (F) between Co_1, Co_2 and Al_2. Adapted from [5].

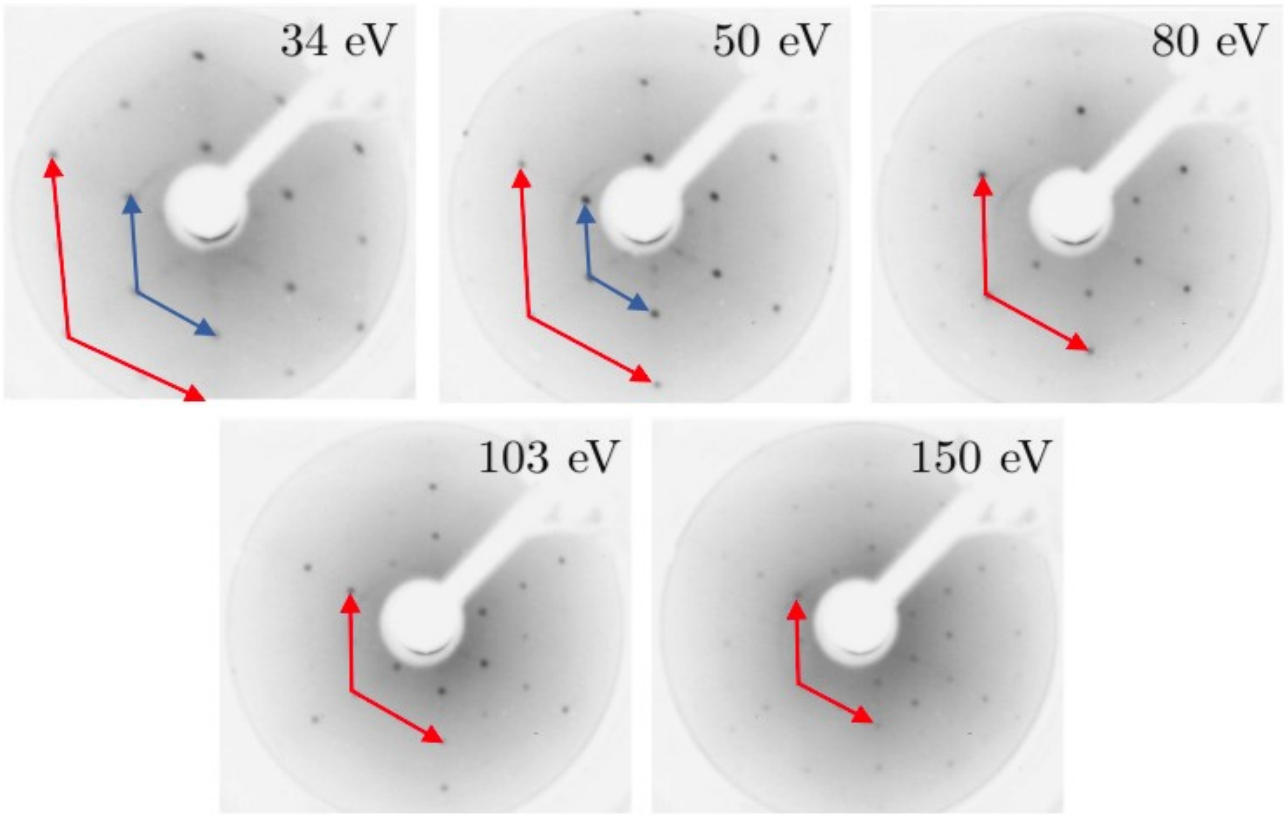

Figure 2: LEED patterns obtained for the energies of 34, 50, 80, 103 and 150 eV for the study of the surface of the Al_5Co_2 (001) compound.

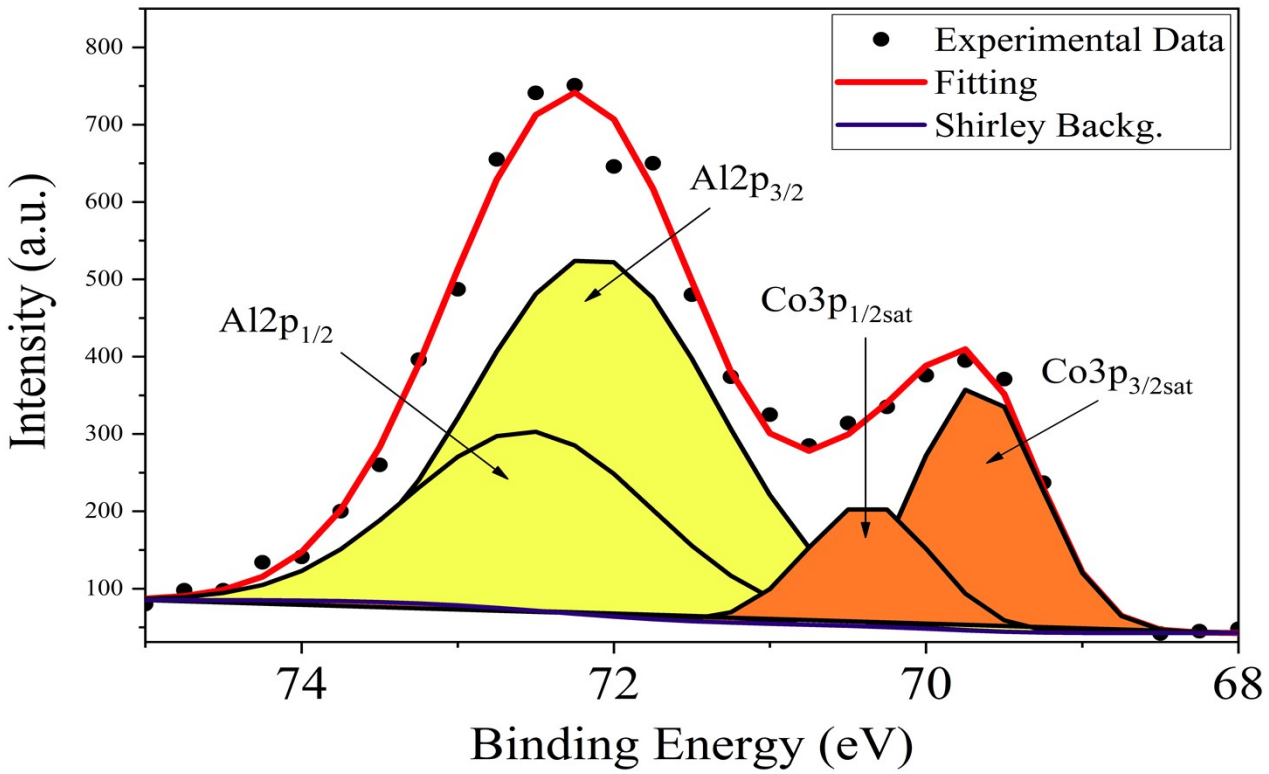

Figure 3: Representation of an Al_5Co_2 XPS spectrum through PED data, containing information on the levels of the Al 2p core with the $2p_{3/2}$ and $2p_{1/2}$ components represented by the color yellow and for the Co 3p satellite with the $3p_{3/2}$ and $3p_{1/2}$ represented by the color orange.

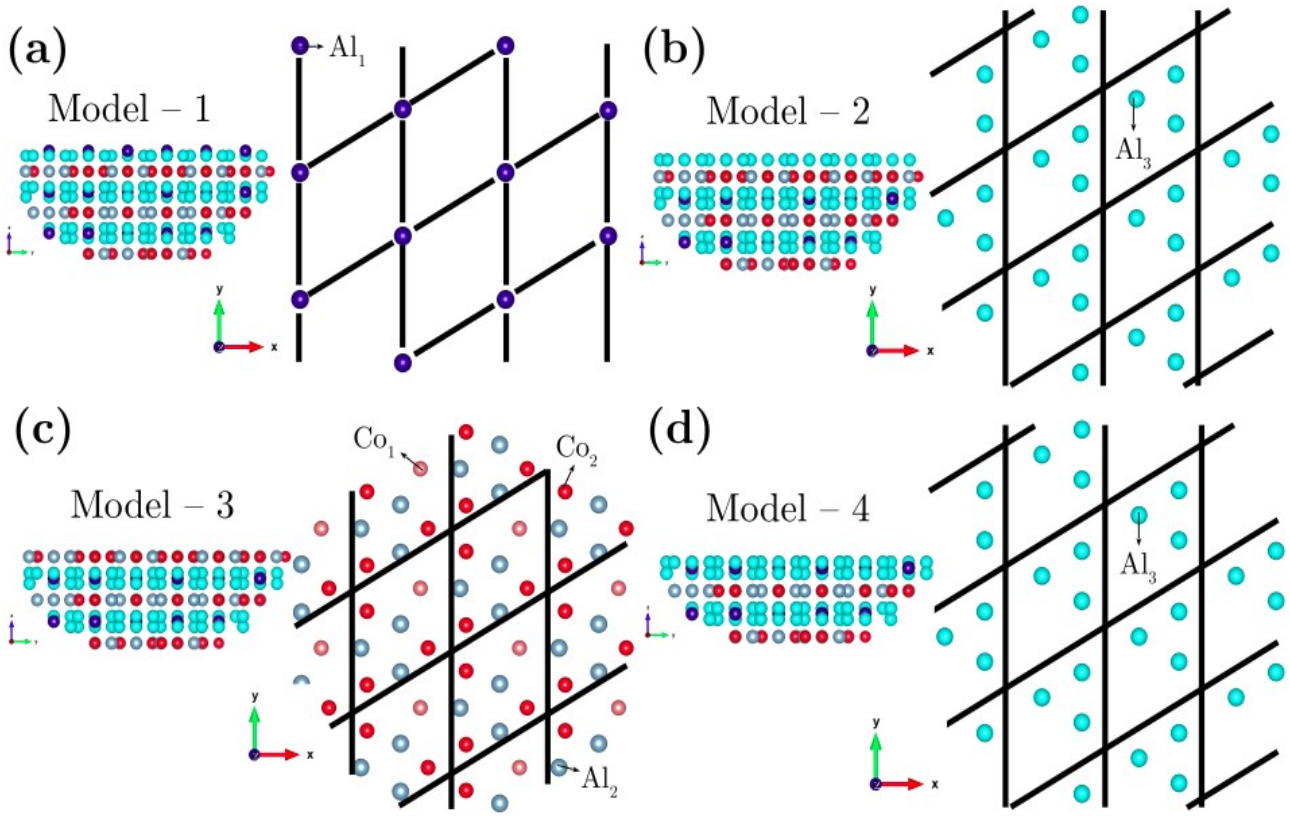

Figure 4: Representation of the 4 cluster models in orientation [001]. The blue and red spheres correspond to Al and Co atoms, respectively.

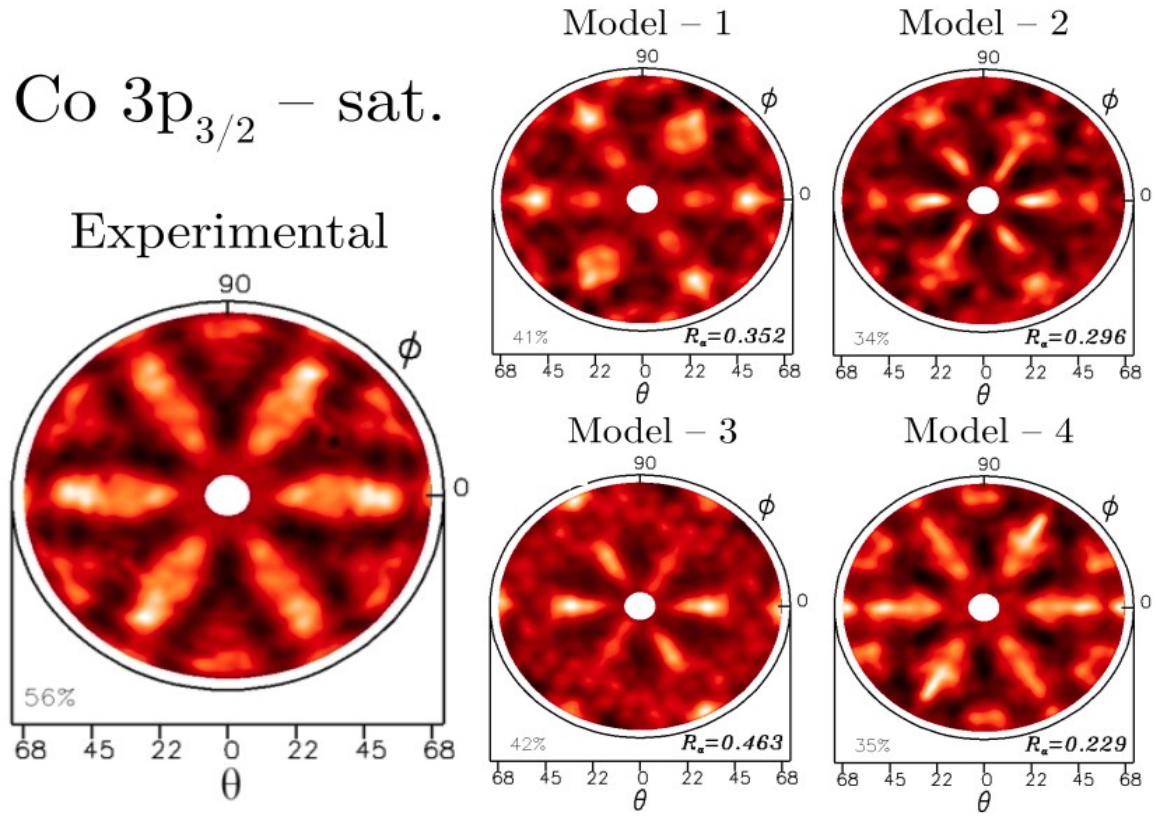

Figure 5: Photoelectron diffraction pattern of the Co $3p_{3/2}$ satellite, excited with 350 eV photons. On the left we have the experimental pattern and on the right the four optimized theoretical models.

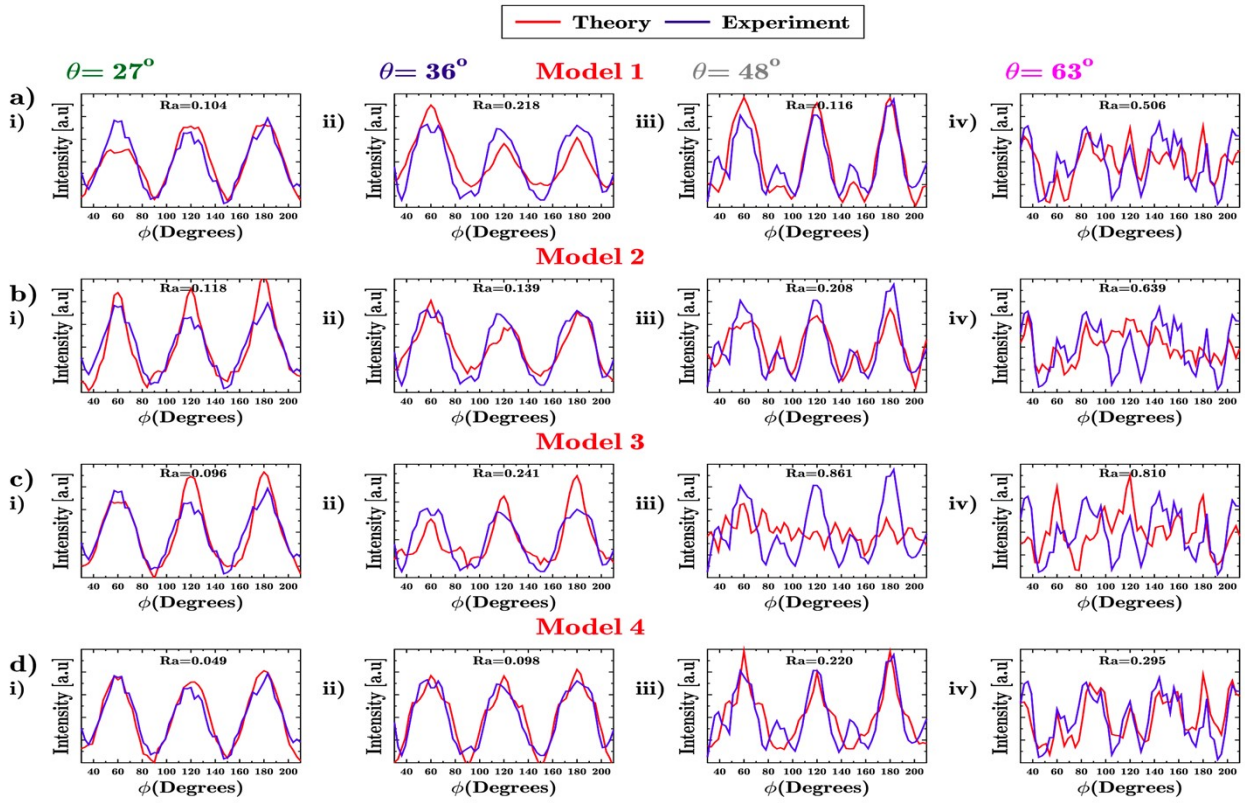

Figure 6: Comparison between simulation, performed using MSCD, and experimental data from PED for four different polar emission angles for Co $3p_{3/2}$ emitting with the 4 models. Red curves indicate MSCD simulation results and blue curves indicate experimental data.

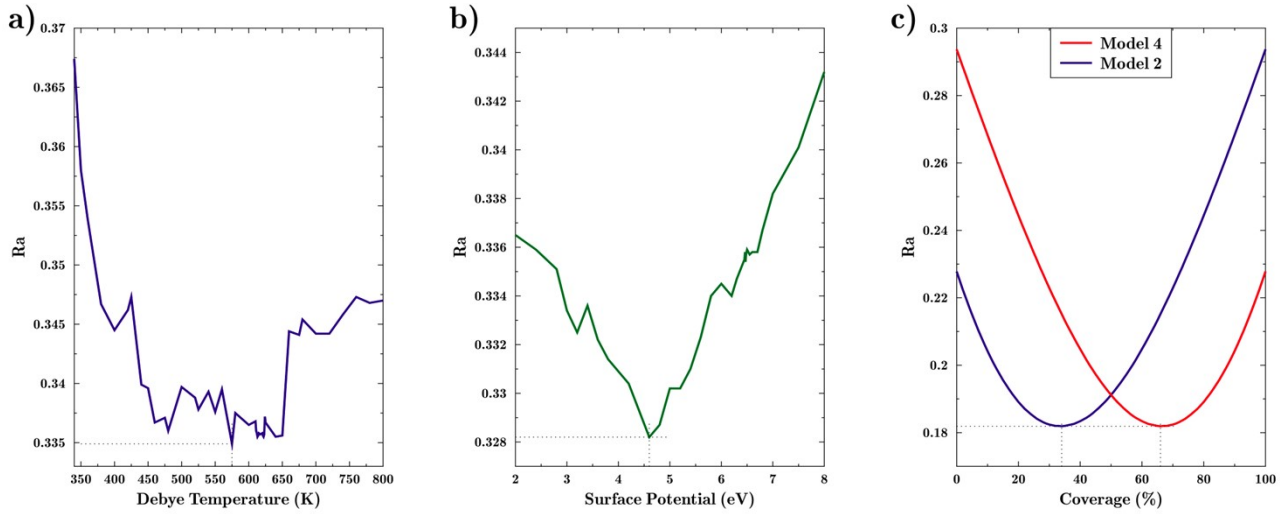

Figure 7: a) Result of R_a optimization as a function Debye Temperature and the best value found was θ_D = 575 K; b) Result of R_a optimization as a function of surface potential (V_0) and the best value found was V_0 = 4.6 eV; c) Result of R_a as a function linear combination between models 2 and 4, in which the best value was for 66% of the model – 4 and 34% of the model – 2.

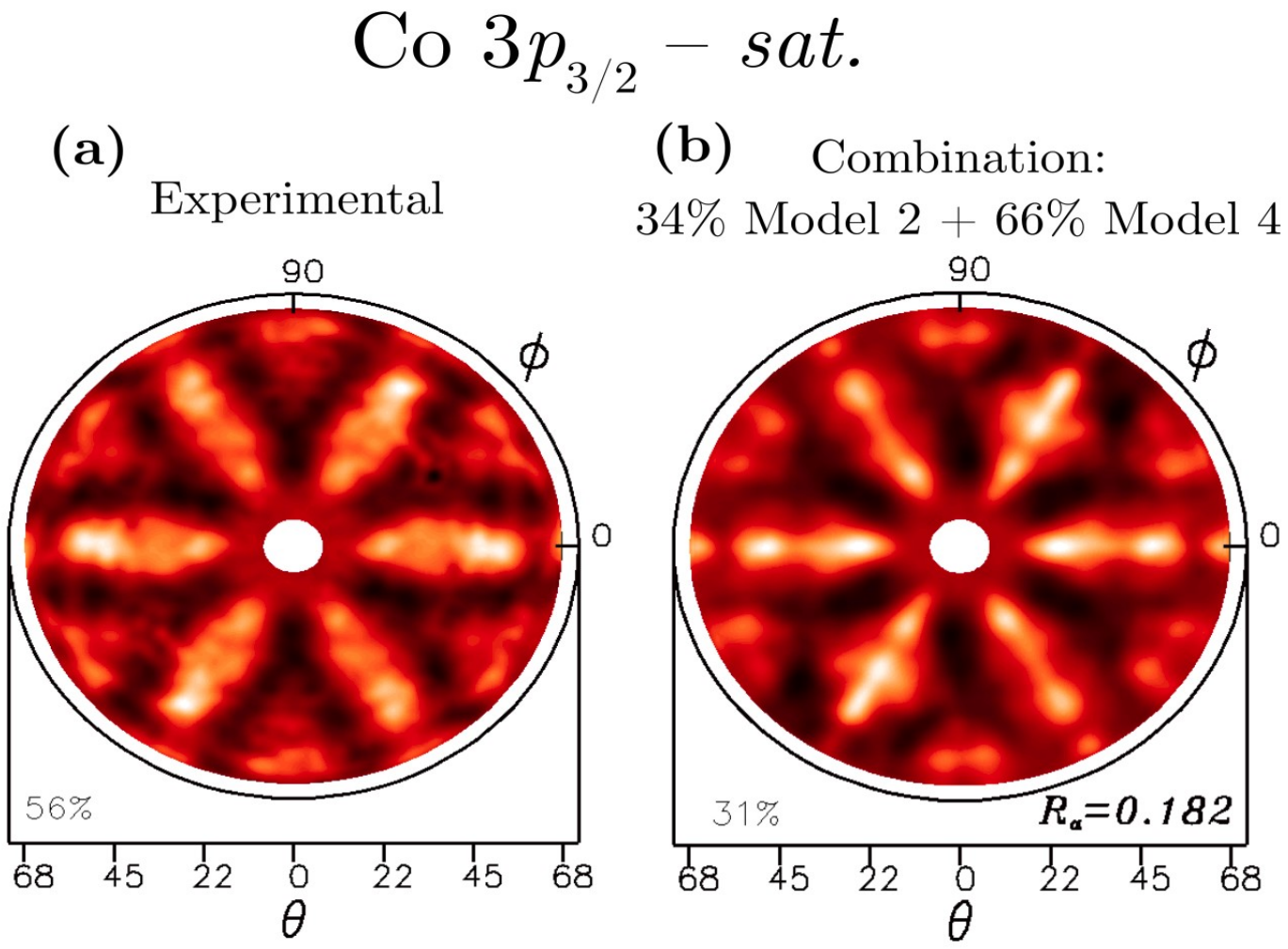

Figure 8: Comparison between the PED standards: (a) Experimental and (b) Theoretical corresponding to the linear combination of the terminations of models 2 and 4 and containing the parameters θ_D = 575 K and V_0 = 4.6 eV.

The figure 9 shows the X-ray photoelectron spectroscopy result after the sputtering and annealing procedures. The spectrum was acquired from a Mg kα source. The surface cleanliness is comproved by the absence of any contaminatiom, maily of the lines os C1s and the O1s.

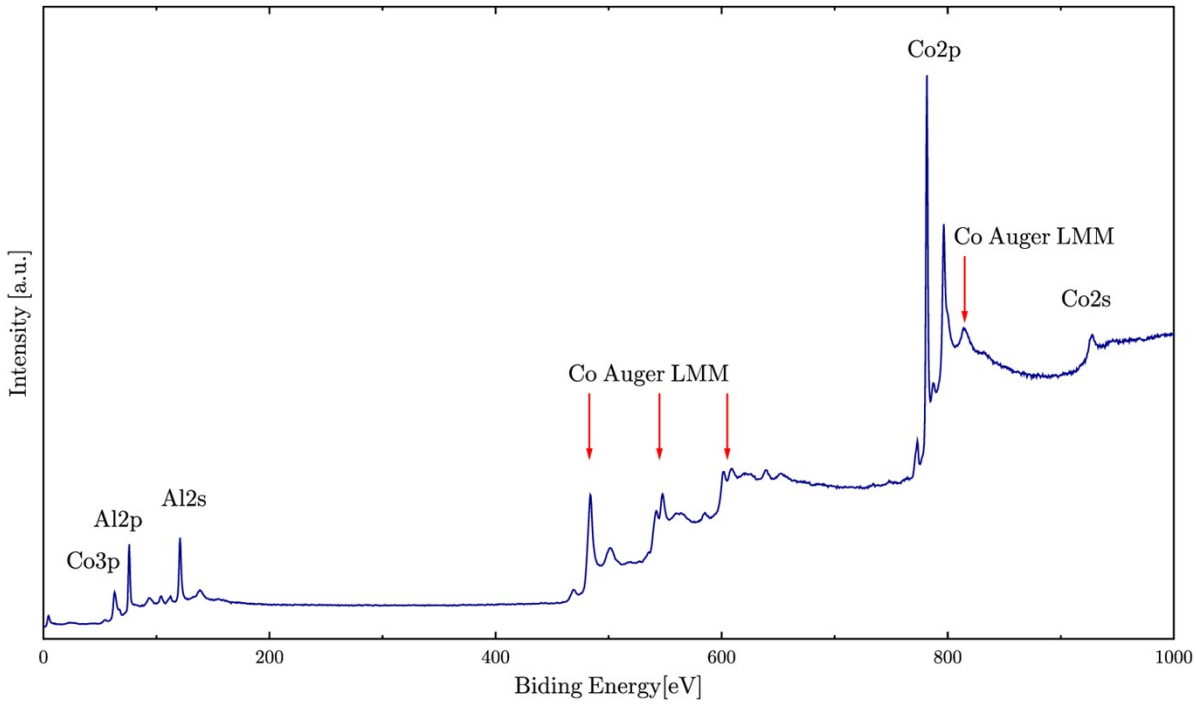

Figure 9: Survey spectrum of the clean surface Al_5Co_2 (001) shown only the elements Al and Co and the total absence of any contamination.