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

Unoccupied Electronic Band Structure of Pentagonal Si Nanoribbons on Ag(110)

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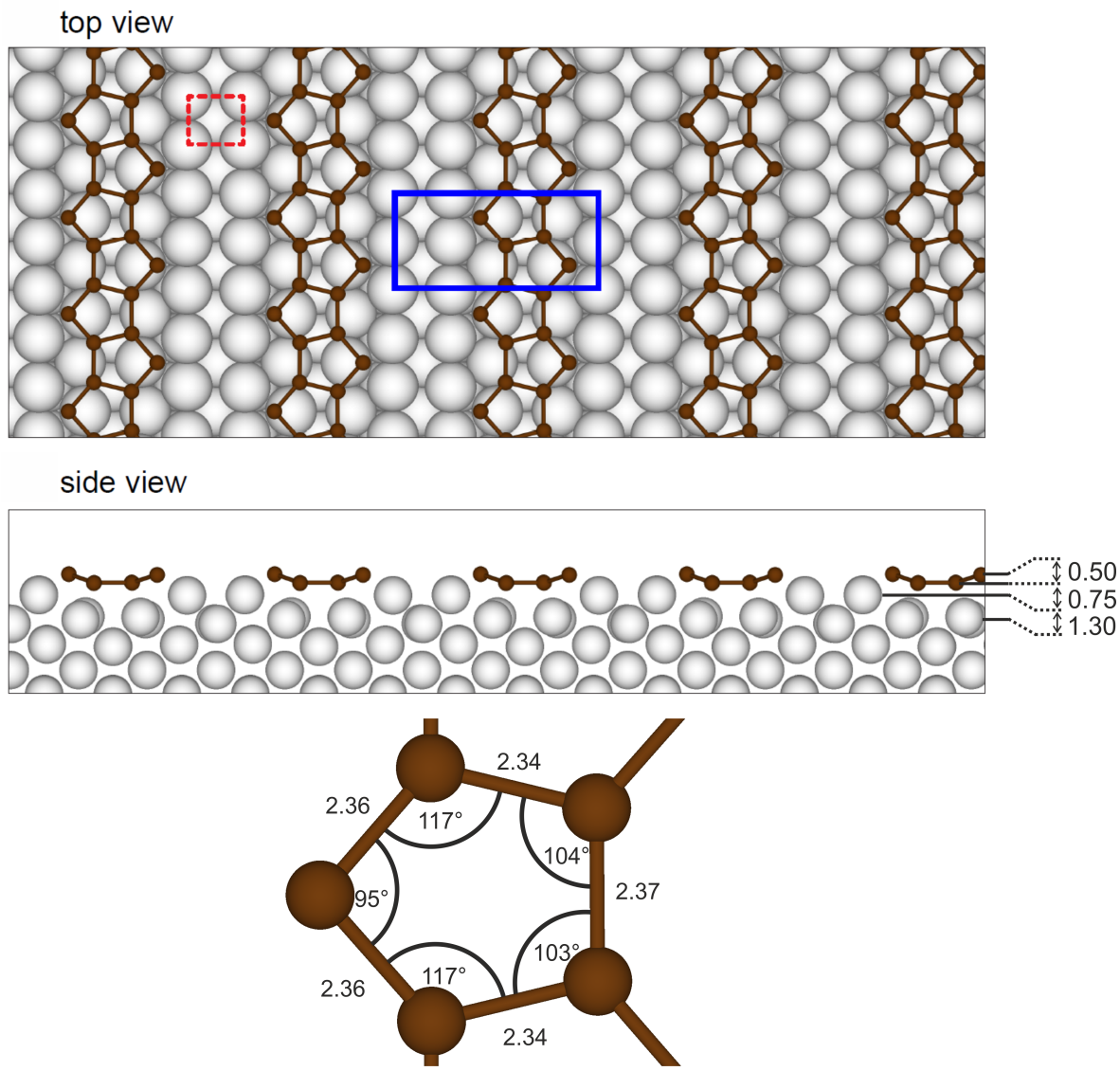

Figure S1: Structural model of the single strand nanoribbons used for the DFT calculations. The red rectangle indicateds the (1×1) unreconstructed Ag(110) unit cell, whereas the blue rectangle indicates the (3×2) reconstruction of the nanoribbons. Measurements of the distances between atoms in the middle and lower panel are given in Å.

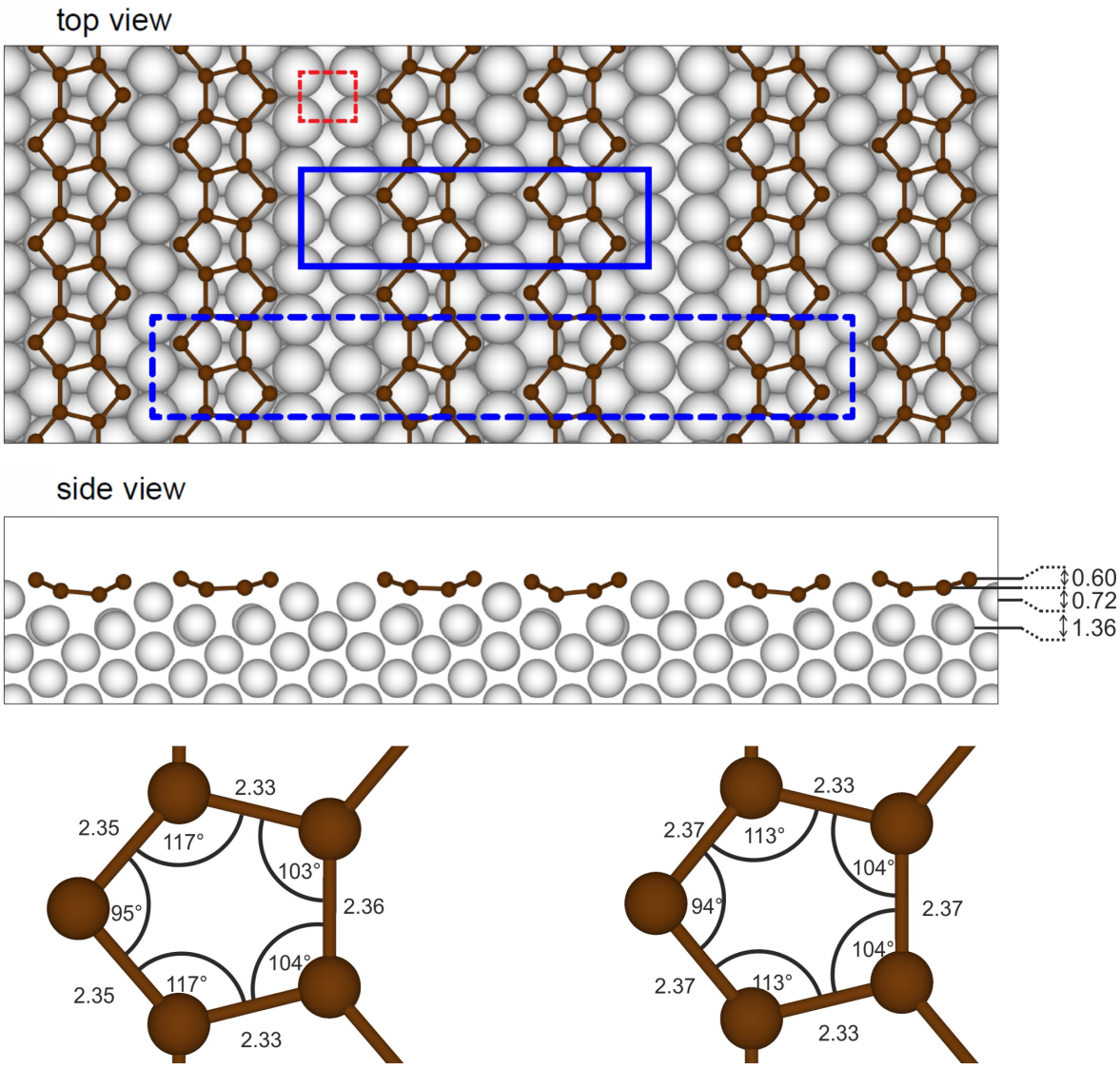

Figure S2: Structural model of the double strand nanoribbons used for the DFT calculations. The red rectangle indicates the (1×1) unreconstructed unit cell of the silver, whereas the blue rectangle indicates the (5×2) reconstruction of Ag(110). The blue dashed rectangle marks the supercell used in the calculations. . Measurements of the distances between atoms in the middle and lower panel are given in Å.

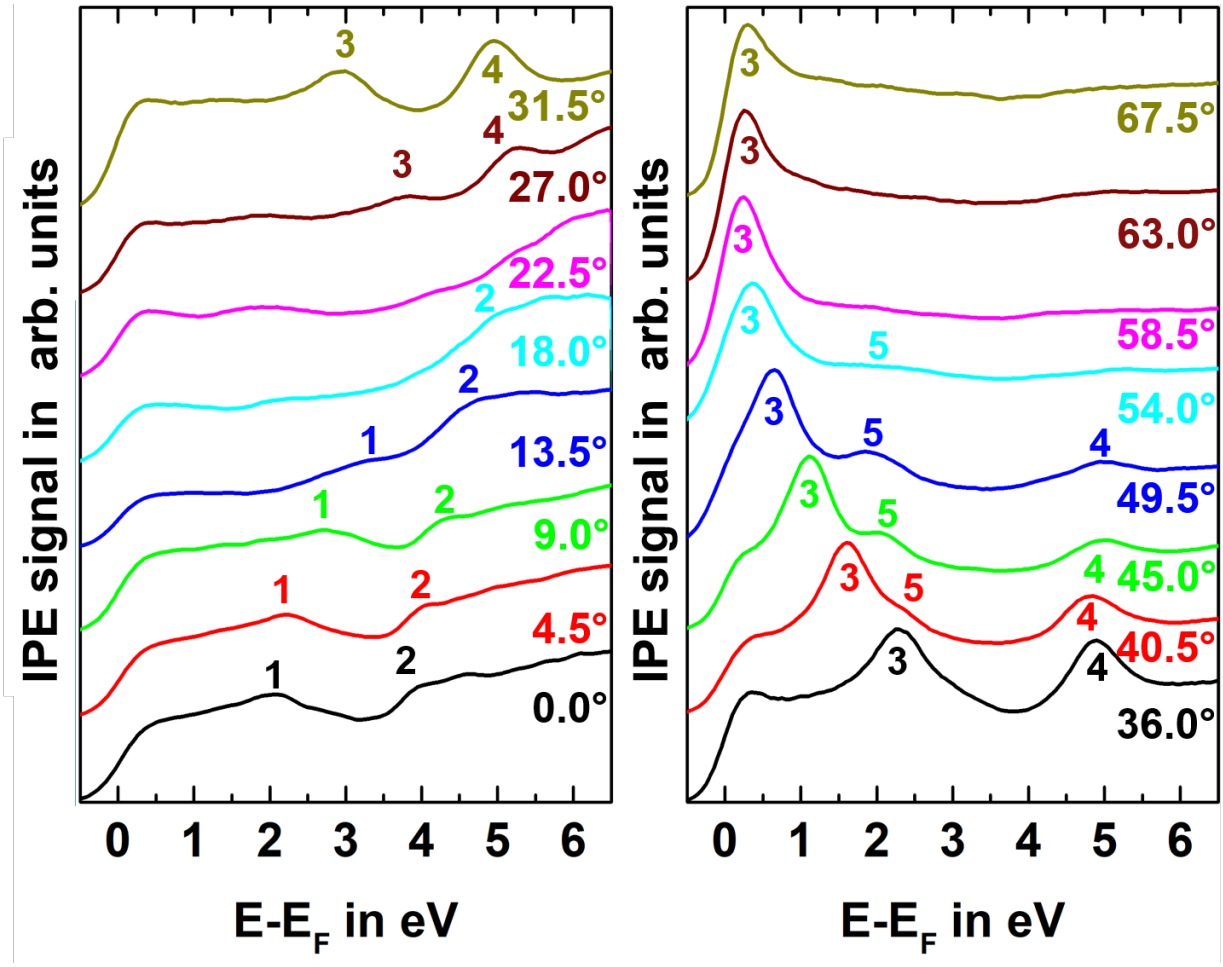

Figure S3: IPE spectra recorded in $\overline{\Gamma X}$ direction on clean Ag(110). Numbers identify the states shown in the band structure in the main manuscript in fig. 1.

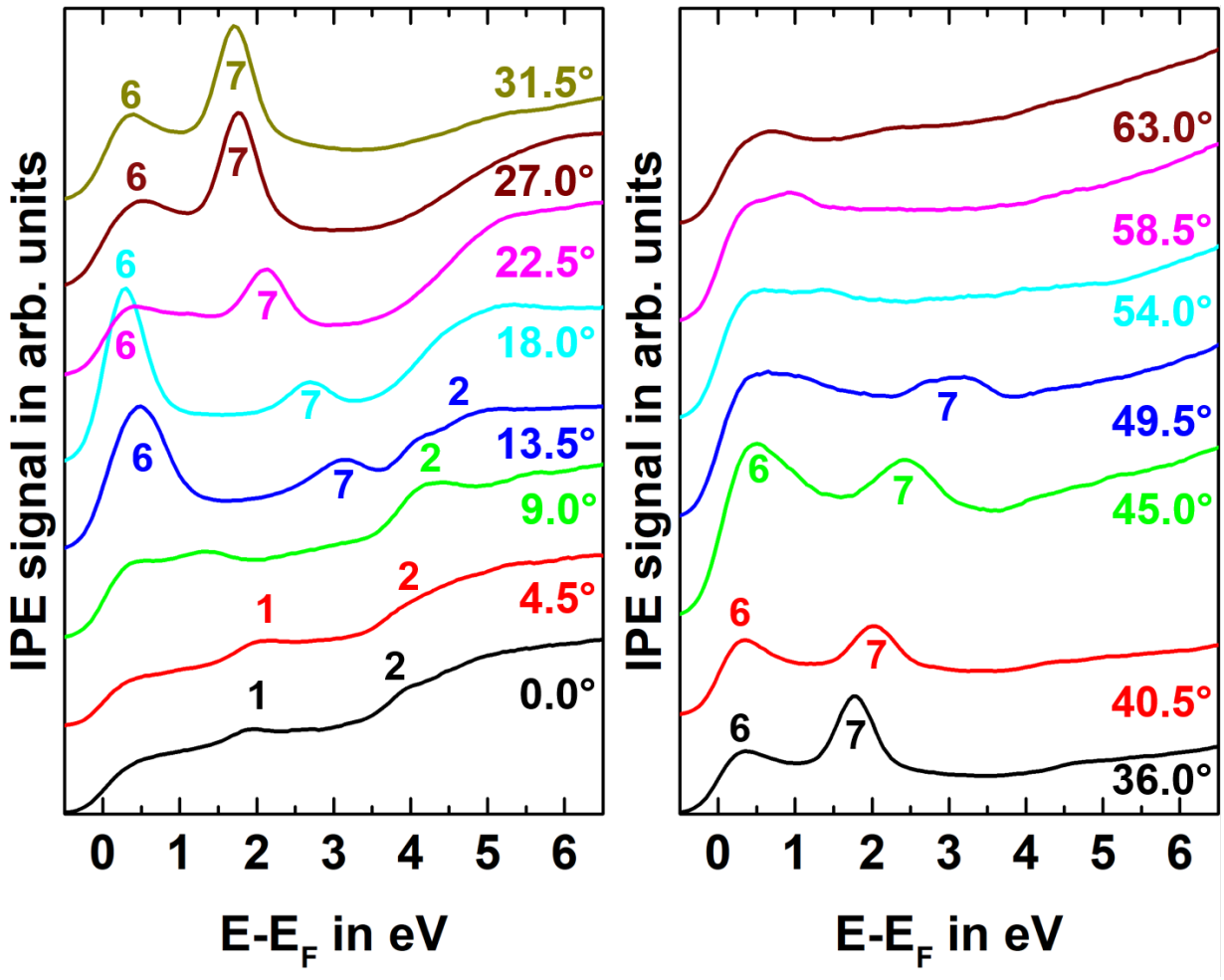

Figure S4: IPE spectra recorded in $\overline{\Gamma Y}$ direction on clean Ag(110). Numbers identify the states shown in the band structure in the main manuscript in fig. 1.

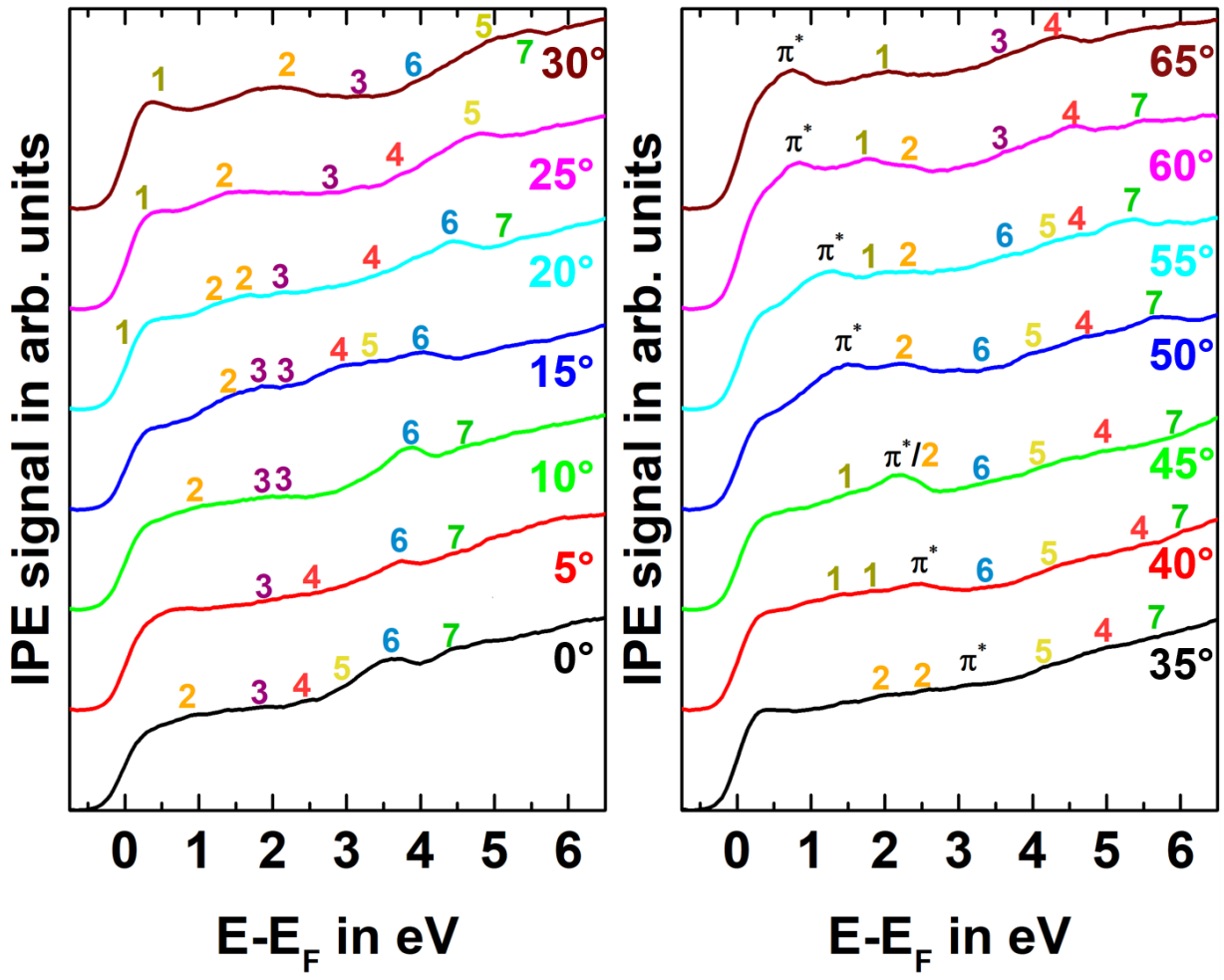

Figure S5: IPE spectra recorded in $\overline{\Gamma X}$ direction (along the nanoribbons) on single strand nanoribbons on Ag(110). The coloured numbers indicate which state in the band structure is associated with the spectral feature in fig 3 of the main manuscript. π^* indicates the peak associated with the overlap of the Ag(110) sp-band and the π^* band of the nanoribbons. Spectra shown are smoothed by a 5-point moving average. States not visible in this depiction are clearly identified when analysing the spectra individually.

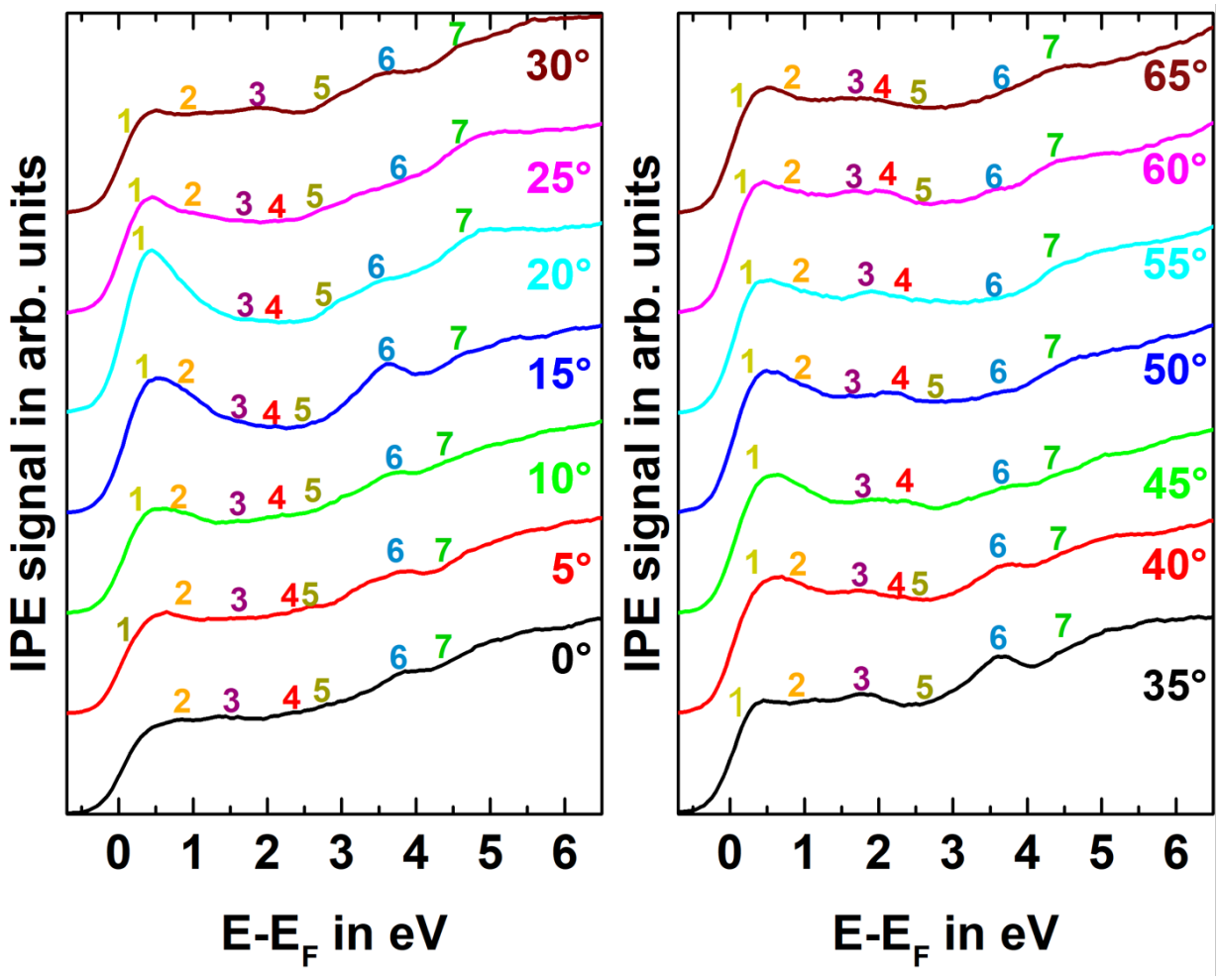

Figure S6: IPE spectra recorded in $\overline{\Gamma Y}$ direction (across the nanoribbons) on single strand nanoribbons on Ag(110). Coloured numbers indicate the assignment of the spectral feature to a state in the band structure in fig. 3 of the main manuscript. Spectra shown are smoothed by a 5-point moving average. States not visible in this depiction are clearly identified when analysing the spectra individually.

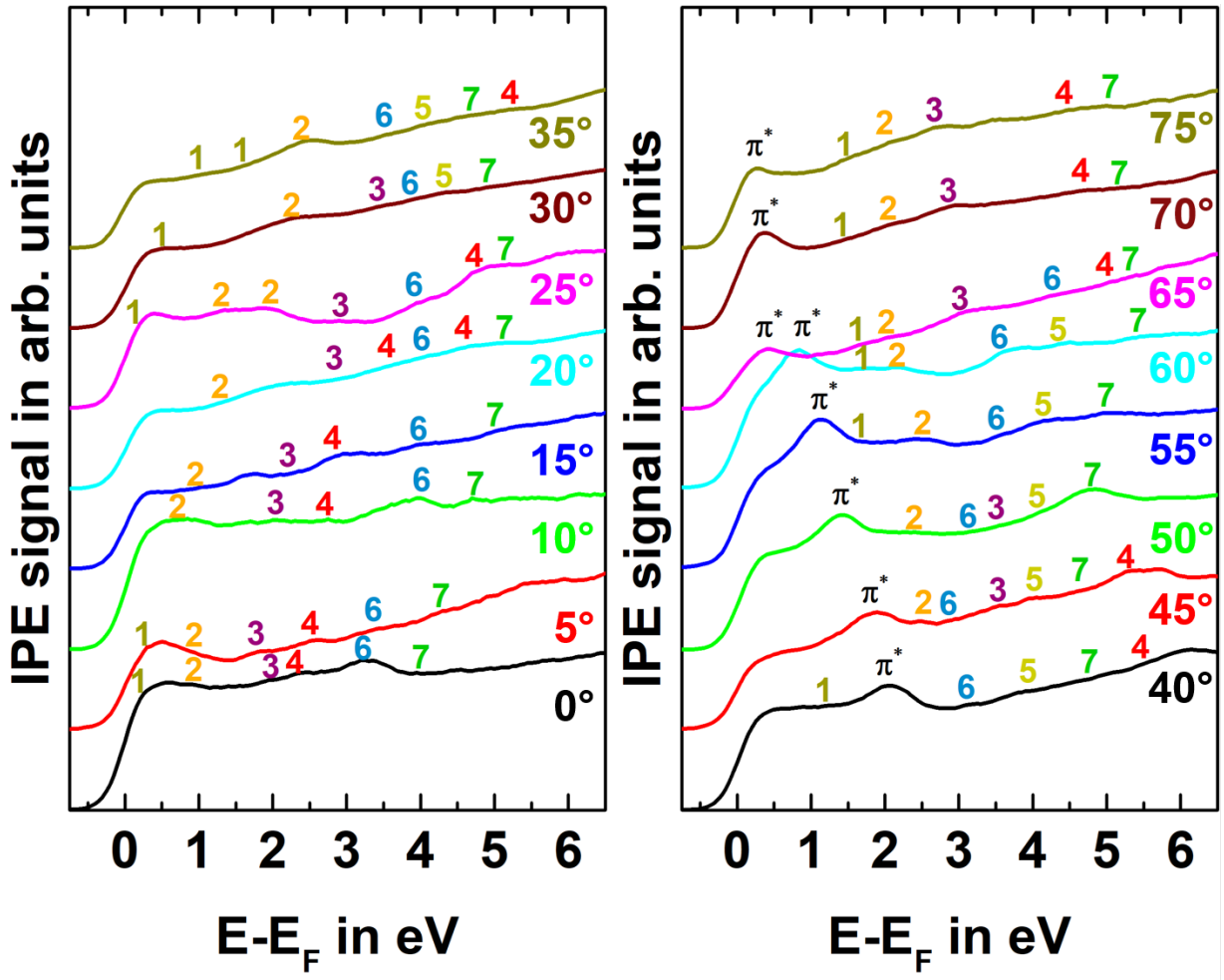

Figure S7: IPE spectra recorded in $\overline{\Gamma X}$ direction (along the nanoribbons) on double strand nanoribbons on Ag(110). The coloured numbers indicate which state in the band structure in fig. 5 of the main manuscript is associated with the spectral feature. π^* indicates the peak associated with the overlap of the Ag(110) sp-band and the π^* band of the nanoribbons.Spectra shown are smoothed by a 5-point moving average. States not visible in this depiction are clearly identified when analysing the spectra individually.

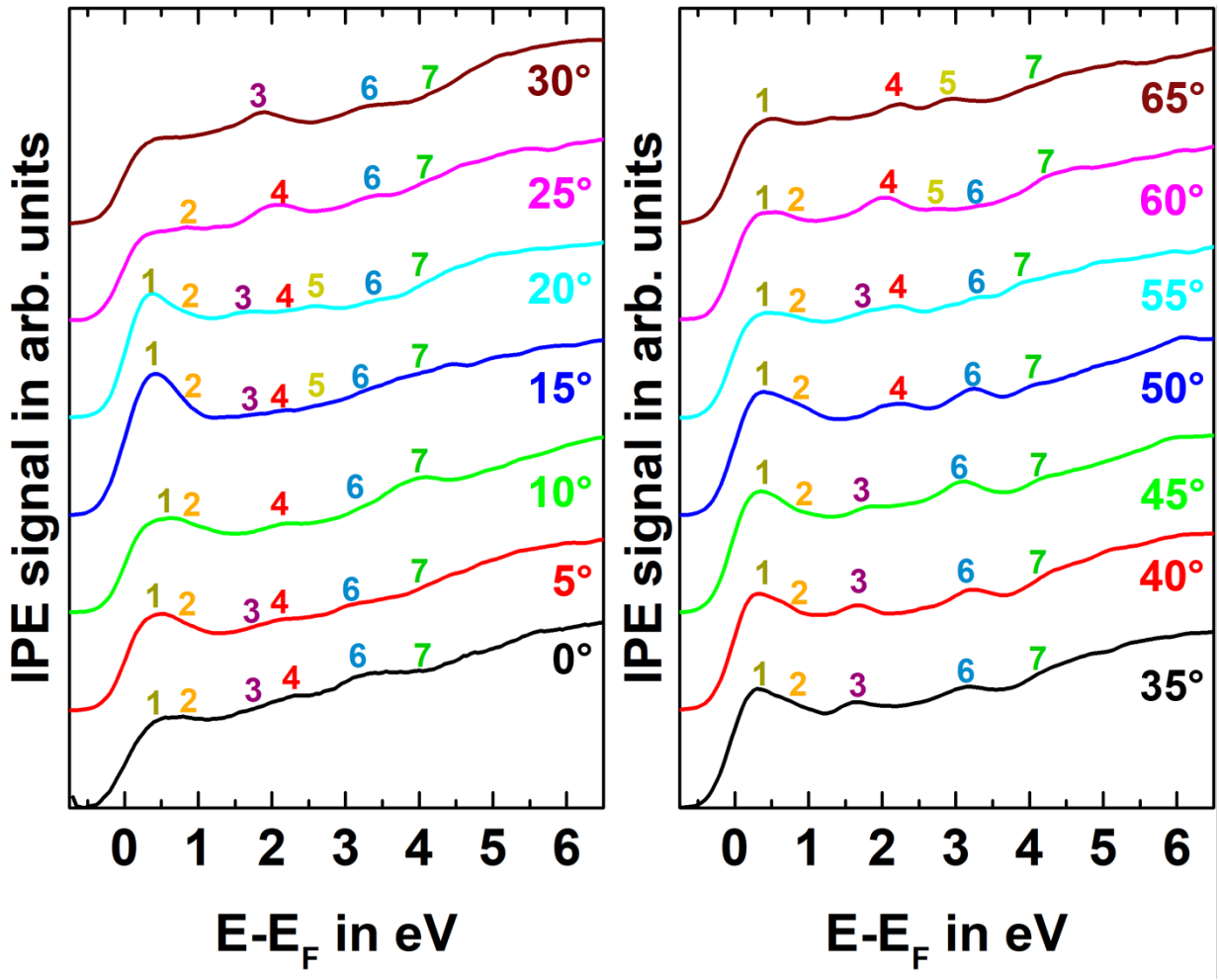

Figure S8: IPE spectra recorded in $\overline{\Gamma Y}$ direction (across the nanoribbons) on double strand nanoribbons on Ag(110). Coloured numbers indicate the assignment of the spectral feature to a state in the band structure in fig. 5 of the main manuscript. Spectra shown are smoothed by a 5-point moving average. States not visible in this depiction are clearly identified when analysing the spectra individually.

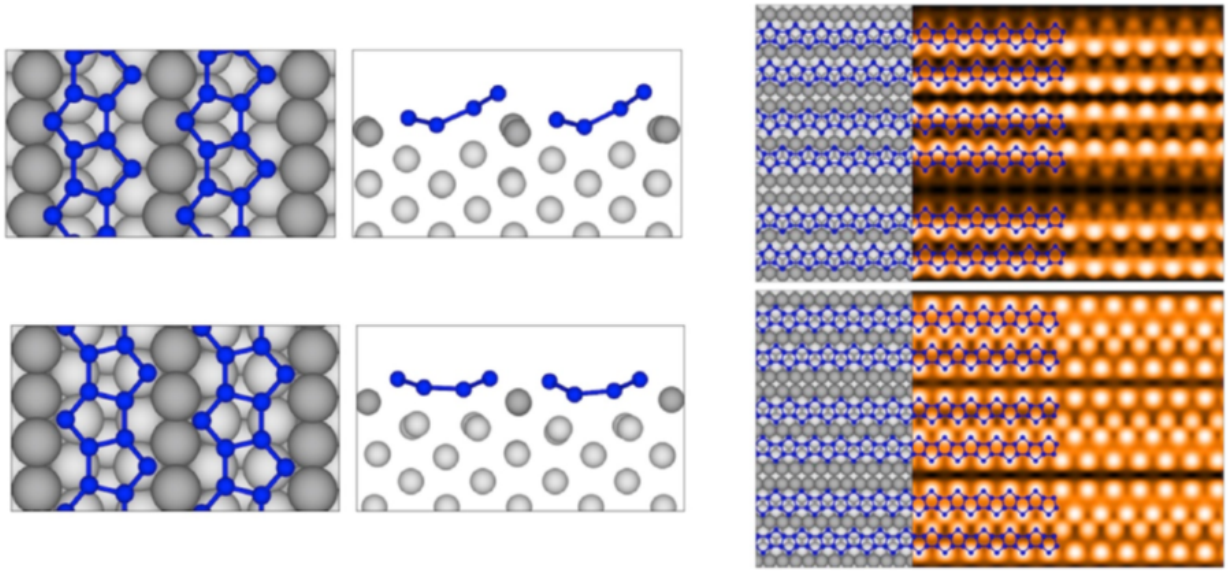

Figure S9: Top panel: DNR model by Espeter *et al.*[1] after relaxation in DFT calculations and corresponding simulated STM image. Lower panel: DNR model used in this study after relaxation and corresponding simulated STM image. The energy of the model in the top panel is 3.6 eV higher per supercell than that of the model in the lower panel. STM images were simulated using the Tersoff-Hamann formalism[2].

References

[1] P. Espeter, C. Keutner, P. Roese, K. Shamout, U. Berges, G. Wenzel, L. Bignardi, N. F. Kleimeier, H. Zacharias and C. Westphal, *Nanotechnology*, 2017, **28**, 455701.

[2] J. Tersoff and D. R. Hamann, *Phys. Rev. B*, 1985, **31**, 805–813.