Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary material for

On the problem of Dirac cones in fullerenes on gold

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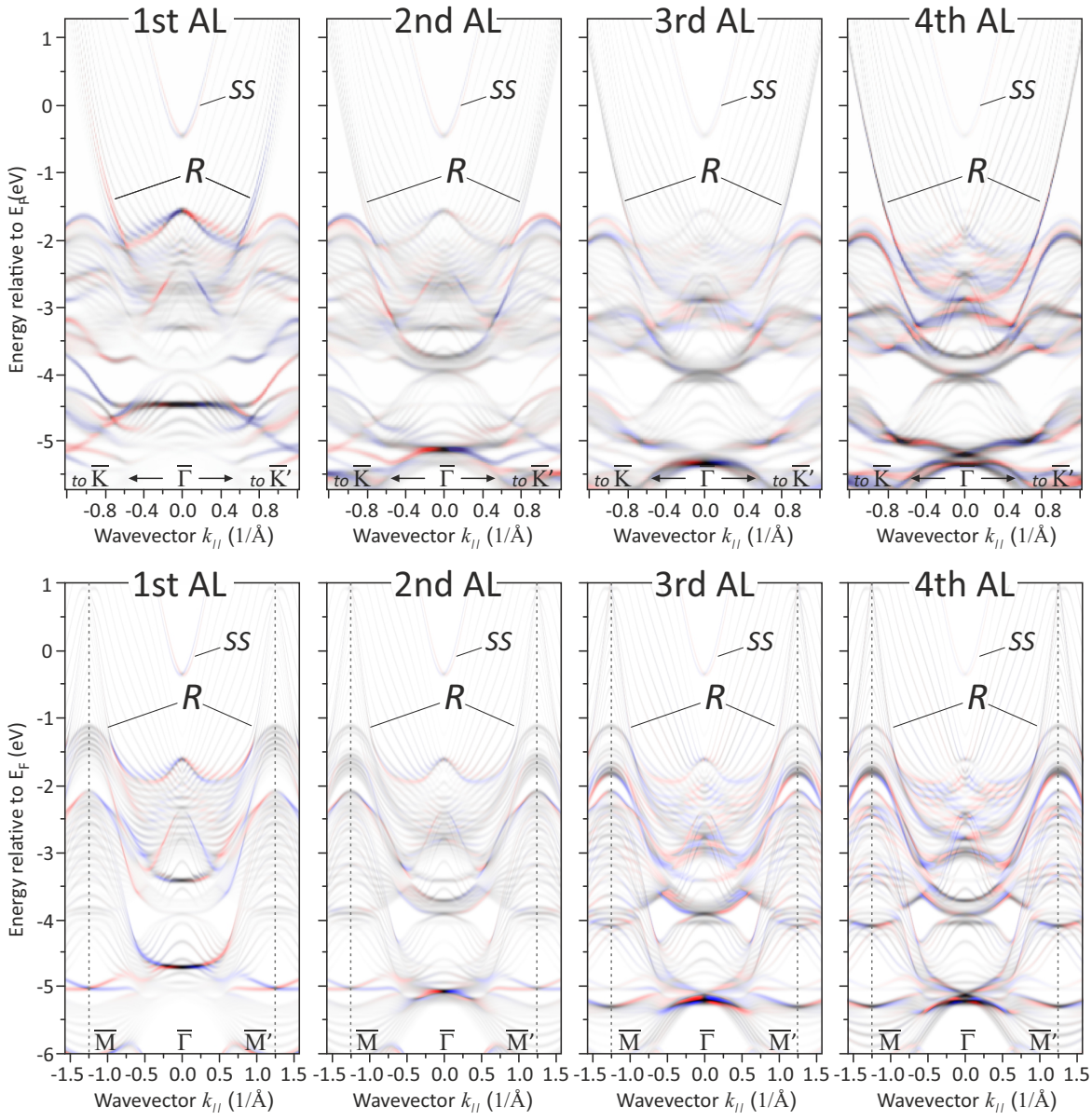

FIG. 1. Layer-resolved DFT of Au(111) [20 ML] in $\overline{\Gamma}-\overline{\mathrm{K}}$ (top) and $\overline{\Gamma}-\overline{\mathrm{M}}$ (bottom) for 1^{st} to 4^{th} atomic layer (AL) with inclusion of spin-orbit interaction. Red and blue colors represent opposite spin projections on the direction normal to the image plane.

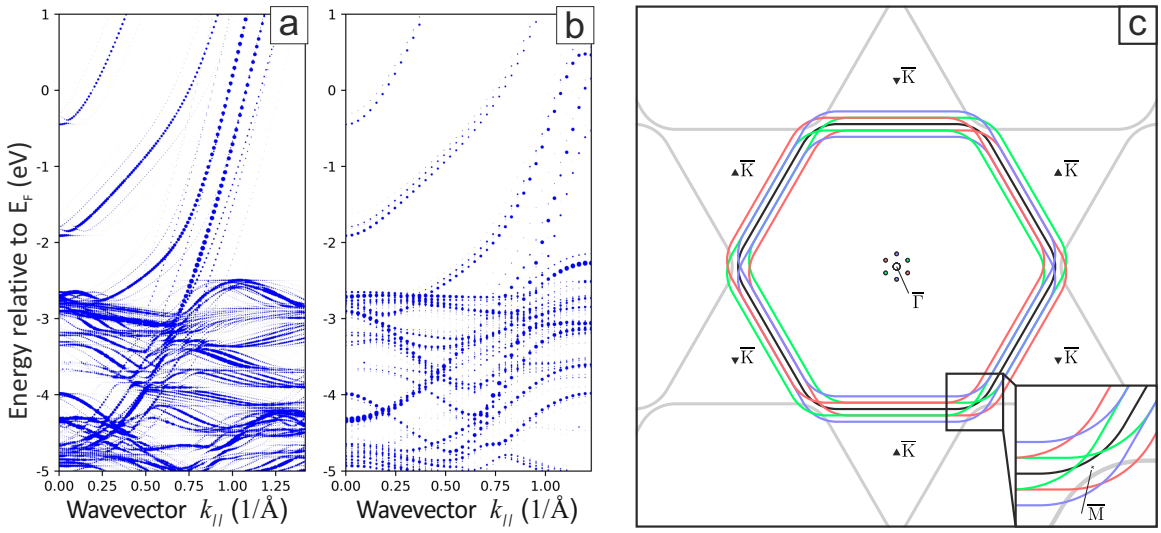

FIG. 2. Effect of Au(111) herringbone ($22 \times \sqrt{3}$) reconstruction on the band structure obtained by DFT calculations. Calculations were performed for a $22 \times \sqrt{3}$ supercell with a 4 ML slab and unfolded to the BZ of gold, projection on the top atomic layer is presented. Both in $\overline{\Gamma} - \overline{\mathrm{K}}$ (a) and $\overline{\Gamma} - \overline{\mathrm{M}}$ (b) directions one can see faint replicas corresponding to the periodicity of the superstructure. Panel (c) demonstrates a sketch of the Au(111) sp-band Fermi contours in the first and neighboring Brillouin zones (shown by black and grey rounded hexagons, respectively) and its first order replicas translated by reciprocal vectors of the herringbone reconstruction in all 6 directions (red, green and blue rounded hexagons, their centers are marked with dots of corresponding color). Length of these vectors is ~ 0.1 Å^{-1}. Inset in the bottom-right corner shows a zoomed-in area around $\overline{\mathrm{M}}$. One can see that the overall pattern of replicas may be very complicated and difficult to distinguish from a single envelope contour in the experiment, especially taking into account their different intensities (see e.g. Ref. 33 from the main text investigating this question for the replicas of the Au(111) surface state).