Simultaneously Understanding the Geometric and Electronic Structure of Anthraceneselenolate on Au(111): A Combined Theoretical and Experimental Study

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MDOS. The molecular density of states is plotted in Figure S1 for all molecular packing arrangements. For this plot, no shifts have been applied (cf., main manuscript)

Figure S1: MDOS plotted for the molecular packing arrangement **A** (solid line), the molecular packing arrangement **B** (dashed line) and the molecular packing arrangement **C** (dotted line).

Bandstructure. The band structure for the SAM bonded to the Au(111) surface is shown in Figure S2. The colored dots represent the projected contribution of the C- and H-Atoms of the molecules onto the entire band structure. Similar to the band structure of the saturated monolayer, the bands arising from the molecular backbone are flat between the $\bar{\Gamma}$ and $\bar{Y}$ points. Between $\bar{\Gamma}$ and $\bar{X}$ a dispersion is observed for the molecular packing arrangements **B** (blue) and **C** (green). Only for **A** (red) the dispersion remains small.

Figure S2: Band structure of the AntSe-SAM bonded to Au(111). The contribution of the molecular backbone (all C- and H-atoms) is shown with coloured dots. Top: molecular packing arrangement **A** (red). Middle: molecular packing arrangement **B** (blue). Bottom: molecular packing arrangement **C** (green).