

Supplementary material for: Spontaneous transmetalation at the ZnPc/Al(100) interface

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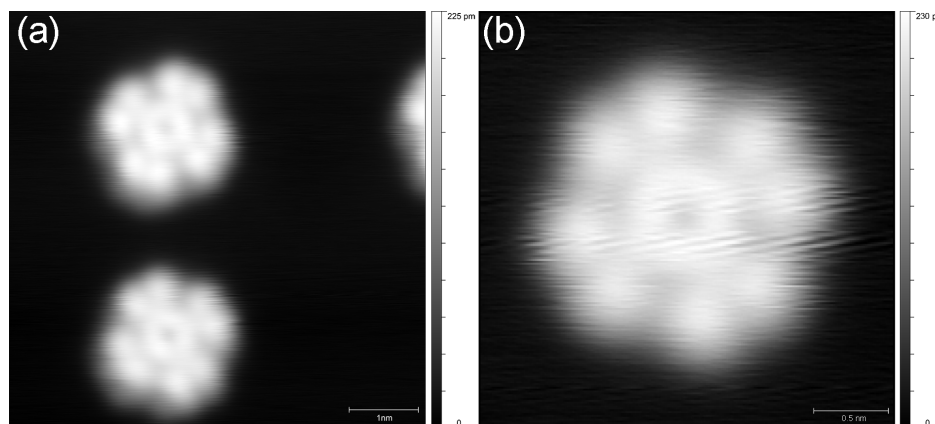


Figure S1: Unfiltered version of STM images contained in figure 5. (a) STM image obtained immediately after deposition ($V=-1.0$ V, $I=1$ nA). Over the molecules the crystallographic directions of Al(100) are superimposed. The figure inset shows the clean Al(100) lattice (b) STM image obtained after annealing to 160 °C ($V=-0.35$ V, $I=50$ pA).

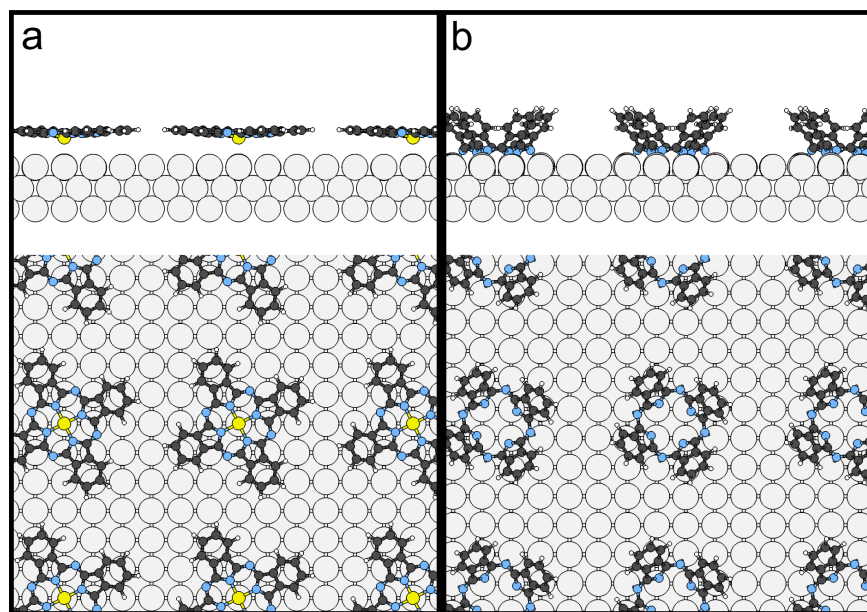


Figure S2: Same as Fig. 1 in the main manuscript, but optimized in a larger 6×6 unit cell. The obtained configurations are nearly indistinguishable from those of the 5×5 unit cell, testifying that the molecular packing is not responsible for the distortion of ·Pc. The norm of displacement vector upon changing from the small to the large cell, $\sqrt{\sum_I |\mathbf{R}_I - \mathbf{R}'_I|^2}$ where \mathbf{R}_I and \mathbf{R}'_I are atomic coordinates in the two cells, amounts to only 0.03 Å in both AlPc and ·Pc cases.