

## Supplementary Material

### Interface Dipoles of Ir(ppy)<sub>3</sub> on Cu(111)

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## STM overview images



Fig. S1 STM overview with low coverage of Ir(ppy)<sub>3</sub> on Cu(111). Image details:  $I = 2$  pA,  $V = 100$  mV. Scale bar 100 Å.

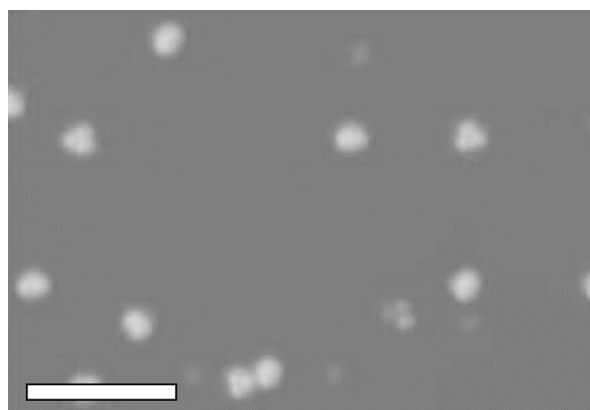


Fig. S2 STM image showing the different alignments of Ir(ppy)<sub>3</sub> on Cu(111). Image details:  $I = 2$  pA,  $V = 50$  mV. Scale bar 100 Å.

## Adsorption angle determination

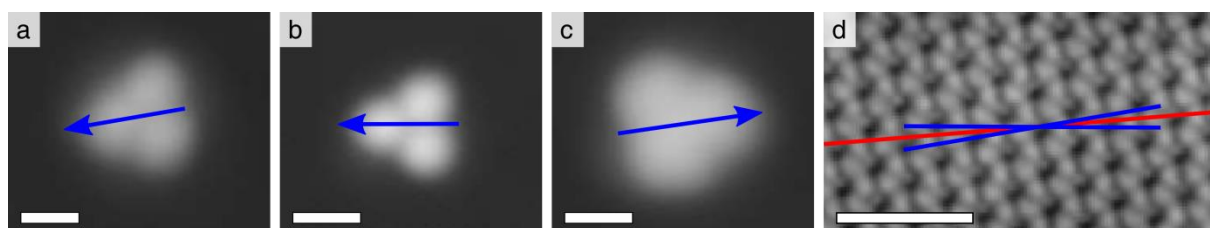


Fig. S3 (a to c) different orientations of Ir(ppy)<sub>3</sub> on Cu(111). (d) Drag-pattern of a Cu adatom on Cu(111), from which the substrate orientation becomes apparent. An analysis of the apparent orientation of 18 different molecules reveals (apart from two outliers) angles of  $\pm 6^\circ$  (a,b) and equivalents (c) with respect to a high-symmetry direction of the underlying Cu(111) substrate (d, red). Image details: (a to c)  $I = 2$  pA,  $V = 0.1$  V; (d)  $I = 2.1$   $\mu$ A,  $V = 0.1$  V. Scale bar 10 Å.