

# Supplementary Materials: Quasi-one-dimensional free-electron-like states selected by intermolecular hydrogen-bonds at the glycine/Cu(100) interface

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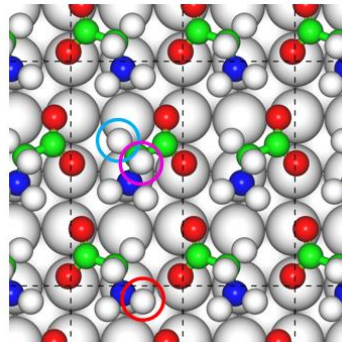
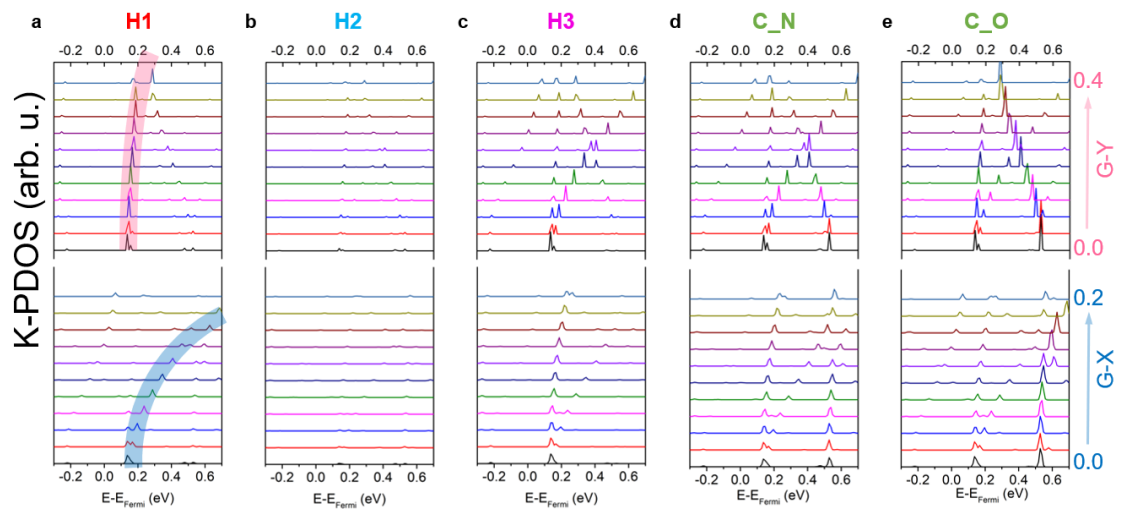


Figure S1. K-resolved local projected density of states ( $kR$ -LPDOS) for other considered atoms. **(a)** the  $kR$ -LPDOS of the H atom marked in red circle (H1), sharing a similar local geometry with H<sub>ani</sub> mentioned in main text, also presents an anisotropic behavior. **(b)** The  $kR$ -LPDOS of the H atom marked in the blue circle (H2), not participating in any hydrogen bond and hybridization with Cu states, shows neglectable DOS projection in the interested range of energy. The H atom marked in the purple circle (H3) **(c)** and those two C atoms both hybridize with the metal surface are not involved in delocalization of molecular state, the  $kR$ -LPDOSs of them **(d,e)** exhibit isotropic projection in both BD-1 and BD-2. Here, C<sub>N</sub> stands for the N-bonding C atom **(d)** and C<sub>O</sub> for the O-bonding one **(e)**, respectively.

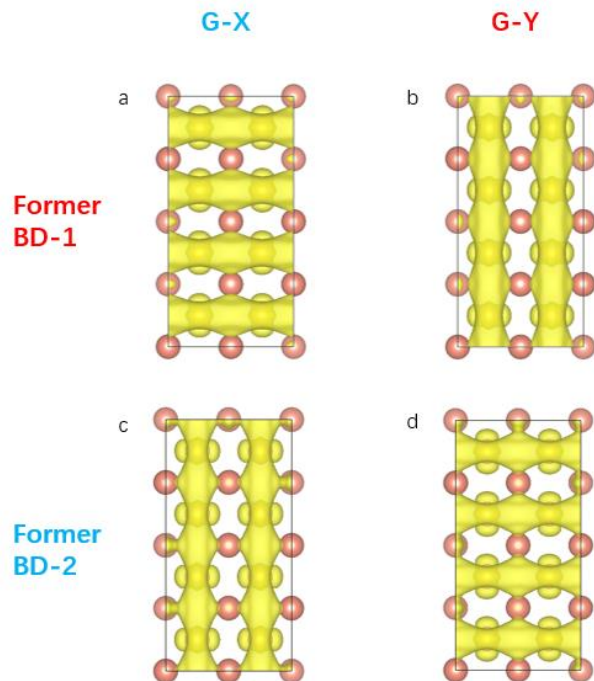


Figure S2. Real space distributions of former p-state in bare Cu surface. Former BD-1 was shown in upper panel (**a,b**), at a point in G-X direction (**a**) and another point in G-Y direction (**b**), respectively. Former BD-2 was shown in lower panel (**c,d**), at a point in G-X direction (**c**) and another point in G-Y direction (**d**). Rather isotropic features (“parallel” and “perpendicular”) were kept in hybridized BD-1 and BD-2.