Suplementry Information for One-dimensional edge state induced by strain in a monolayer copper nitride on Cu(001)

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Figure 9S Band calculation results with projections to subsurface Cu $4p$ orbitals

Fig. 1S *dI/dV* mapping showing the edge state

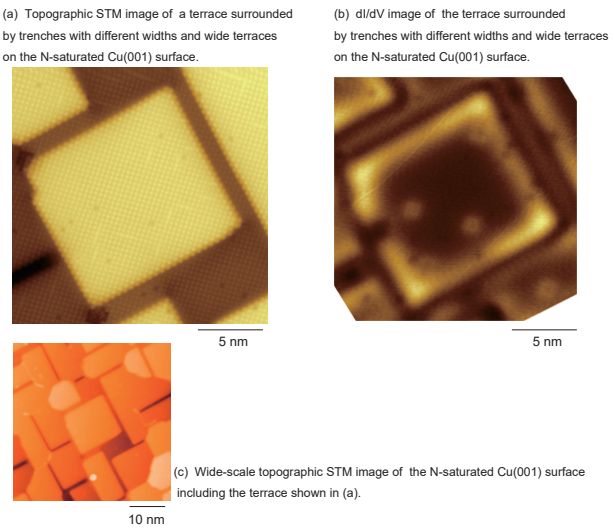

Fig. 1 (a) STM image of a N-saturated Cu(001) surface. Sample bias voltage (V_B) is − 0.1 V. The central terrace has step edges to the lower terraces with different widths. Wide scale STM image including this terrace is shown in (c). (b) dI/dV mapping on the surface including the central terrace shown in (a). (V_B = 2.1 V) At this bias voltage, LDOS is large near the step edge, showing the presence of the one-dimensional step edge states irrespective of the width of the lower terrace. (c) Wide-scale STM image including the terrace shown in (a). (V_B = 1 V). The central terrace in this image is the same as that in (a).

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Fig. 2S Comparisons of LDOS

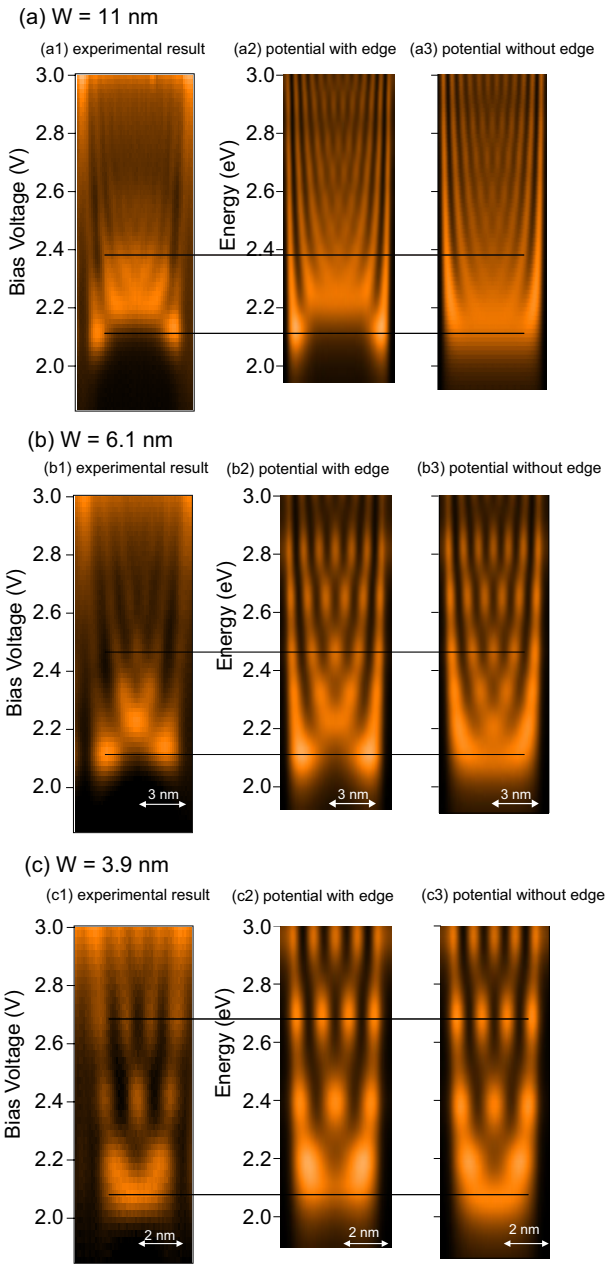

Fig. 2 Comparison of the experimental results with the results of LDOS calculations for 11 (a), 6.1 (b), and 3.9 nm (c) wide terraces. Horizontal lines are guides for the eye. (a1, b1, c1) experimental results. (a2, b2, c2) LDOS calculations for the potential with the edge potential. (a3, b3, c3) LDOS calculations for the potential without the edge potential.The potential parameters are common to the results shown in Fig. 3(a) of the main text except $D_{\mathrm{E}} = 0$ eV for (a3, b3, c3).

Fig. 3S Standing wave in the edge potential

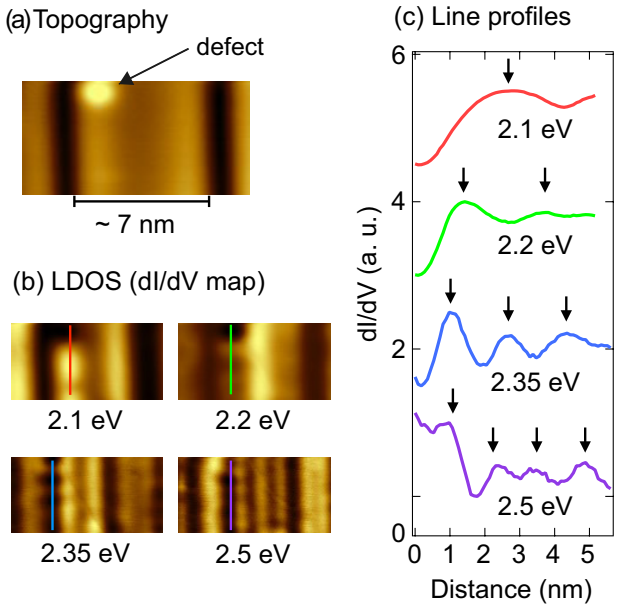

Fig. 3 (a) STM image of a N-saturated Cu(001) surface with two trenches and a defect at the step edge. (b) dI/dV mappings on the surface including the defect in (a), showing standing waves in the both directions perpendicular and parallel to the step edges at constant V_{B} values given in the figure. One-dimensional standing wave parallel to the step edge is seen only near the defect. (c) Line profiles of the standing waves along the lines in (b). The effective mass of the electrons confined in the edge potential evaluated from the line profiles and dispersion relation is $0.22 m_e$.

Fig. 4S Band calculation results with projections to N orbitals

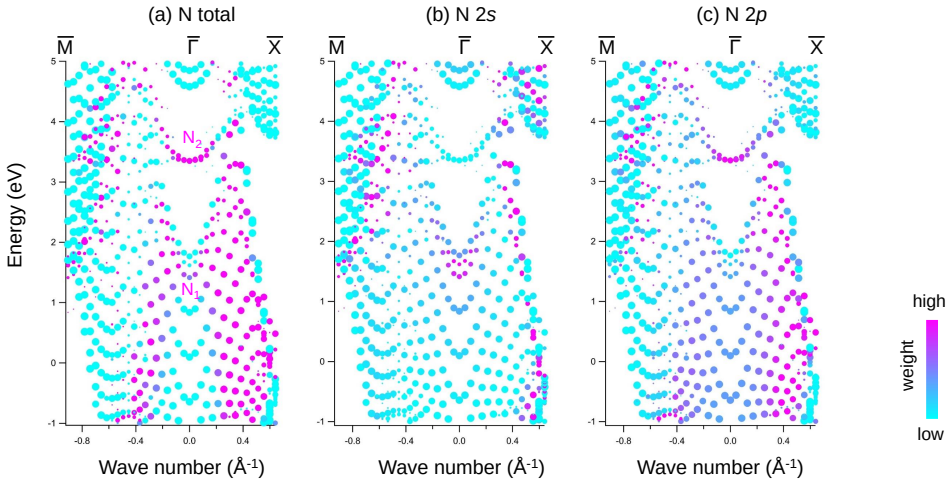

Fig. 4 Calculated band structure of the N-adsorbed Cu(001) slab model with projections to the N orbitals. The circle radius indicates the spectral weight. The weight of the N orbitals is shown as a color gradient. (a) projection to both $2s$ and $2p$ orbitals (b) projection to $2s$ orbital, and (c) projection to $2p$ orbital.

Fig. 5S Band calculation results with projections to surface Cu orbitals

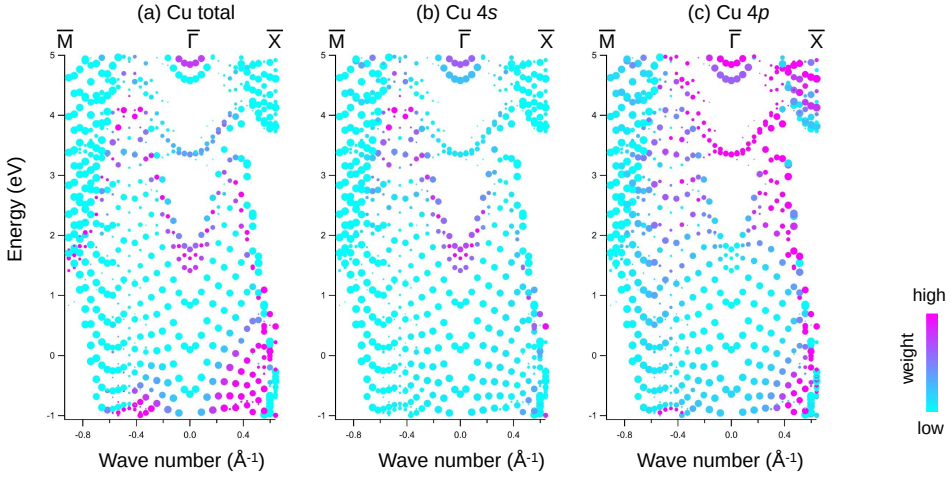

Fig. 5 Calculated band structure of the N-adsorbed Cu(001) slab model with projections to the orbitals of the surface Cu atoms. The circle radius indicates the spectral weight. The weight of the Cu orbitals is shown as a color gradient. (a) projection to both $4s$ and $4p$ orbitals (b) projection to $4s$ orbital, and (c) projection to $4p$ orbital.

Fig. 6S Band calculation results with projections to subsurface Cu orbitals

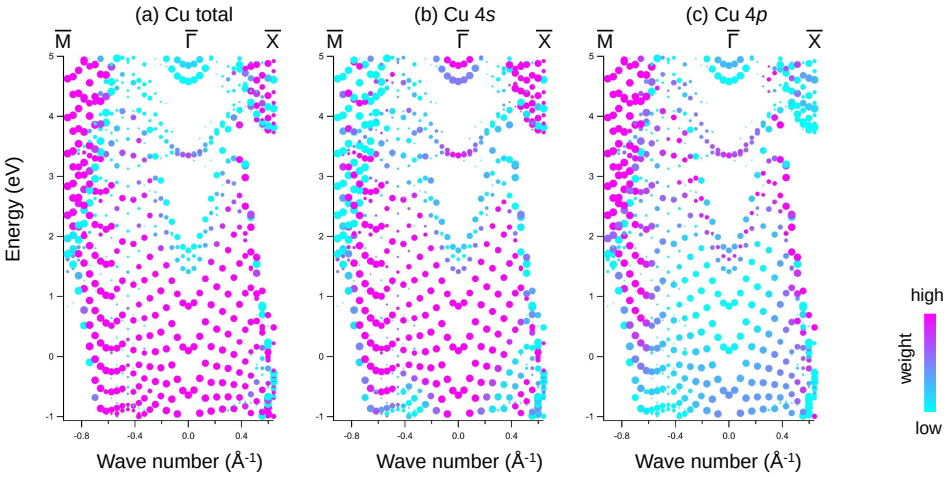

Fig. 6 Calculated band structure of the N-adsorbed Cu(001) slab model with projections to the orbitals of the subsurface Cu atoms. The circle radius indicates the spectral weight. The weight of the Cu orbitals is shown as a color gradient. (a) projection to both 4s and 4p orbitals (b) projection to 4s orbital, and (c) projection to 4p orbital.

Fig. 7S Band calculation results with projections to N 2p orbitals

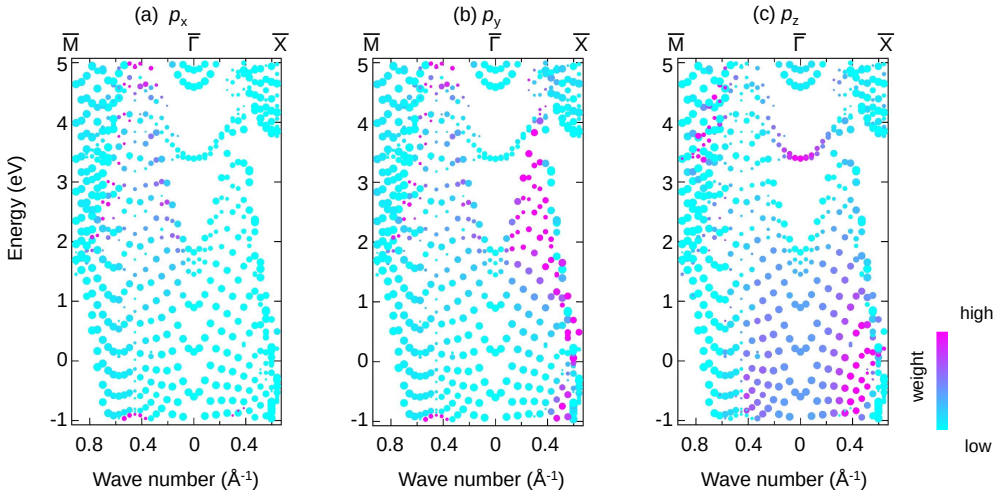

Fig. 7 Calculated band structure of a slab model of N-adsorbed Cu(001) with projections to the N 2p_x (a), N 2p_y (b) and N 2p_z (c) orbitals. The circle radius indicates the spectral weight. The weight of the orbitals is shown as a color gradient.

Fig. 8S Band calculation results with projections to surface Cu 4*p* orbitals

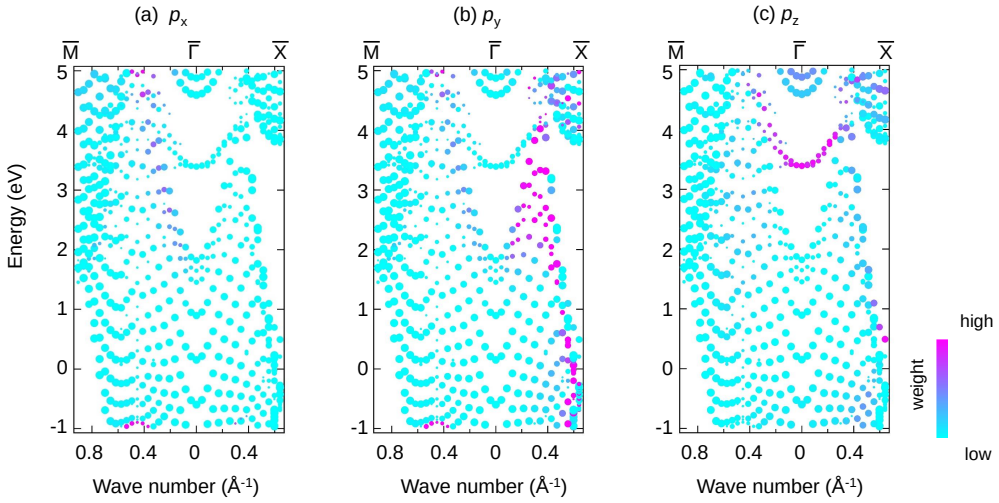

Fig. 8 Calculated band structure of a slab model of N-adsorbed Cu(001) with projections to the surface $4p_x$ (a), $4p_y$ (b) and $4p_z$ (c) orbitals. The circle radius indicates the spectral weight. The weight of the orbitals is shown as a color gradient.

Fig. 9S Band calculation results with projections to subsurface Cu 4*p* orbitals

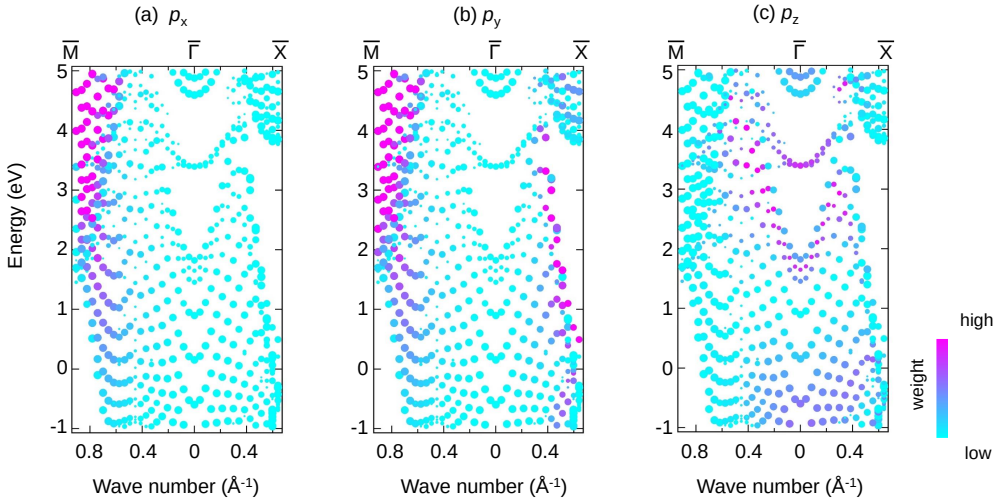

Fig. 9 Calculated band structure of a slab model of N-adsorbed Cu(001) with projections to the subsurface $4p_x$ (a), $4p_y$ (b) and $4p_z$ (c) orbitals. The circle radius indicates the spectral weight. The weight of the orbitals is shown as a color gradient.