Supporting Information for

Experimental Realization of One-Dimensional Metal-Inorganic Chain: Gold-Phosphorus Chain

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Figure S1 displays the atomic model of the magic P_4 cluster.

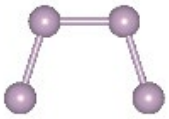

Figure S1. Atomic model of P_4 cluster.

Figure S2a is the STM image of the clean Au(110), with a typical (2 × 1) surface reconstructed pattern. The crystallographic directions of the Au(110) surface are indicated by the red arrows and the lattice distance measured along the [001] direction is 0.8 nm, as revealed by the line profile in Figure S2b.

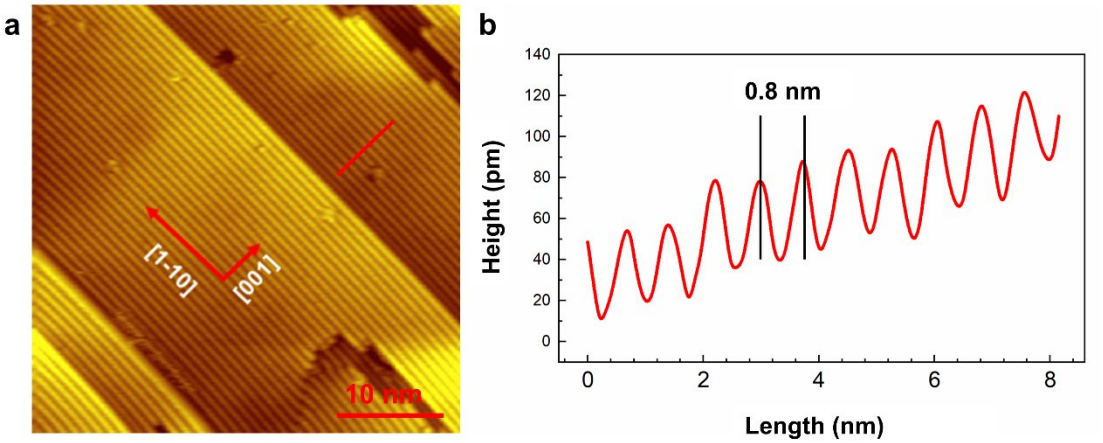

Figure S2. (a) STM image of the clean Au(110) with (2 × 1) reconstruction (V_s = 300 mV, 40 × 40 nm^2). The crystallographic directions of Au(110) surface are indicated by the red arrows. (b) Lateral profile measured along the line in Figure S2a.

Figure S3 shows the Au 4f spectrum for the clean Au(110) surface, where the peak can be fitted by two components located at 83.7 eV and 84.0 eV, corresponding to the surface gold atoms and the bulk gold atoms, respectively.

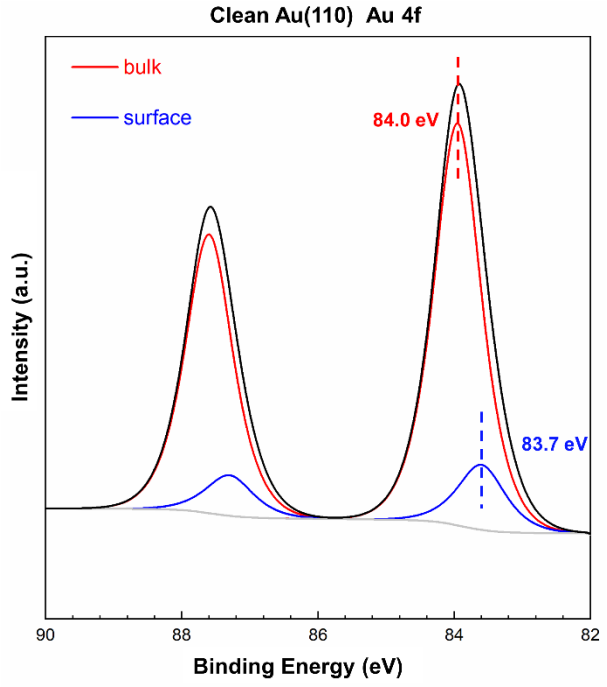

Figure S3. XPS core level spectrum of Au 4f for the clean Au(110).

Figure S4 shows the P 2p spectrum for the clean bulk black phosphorus and the P $2p_{3/2}$ peak is located at 129.9 eV.

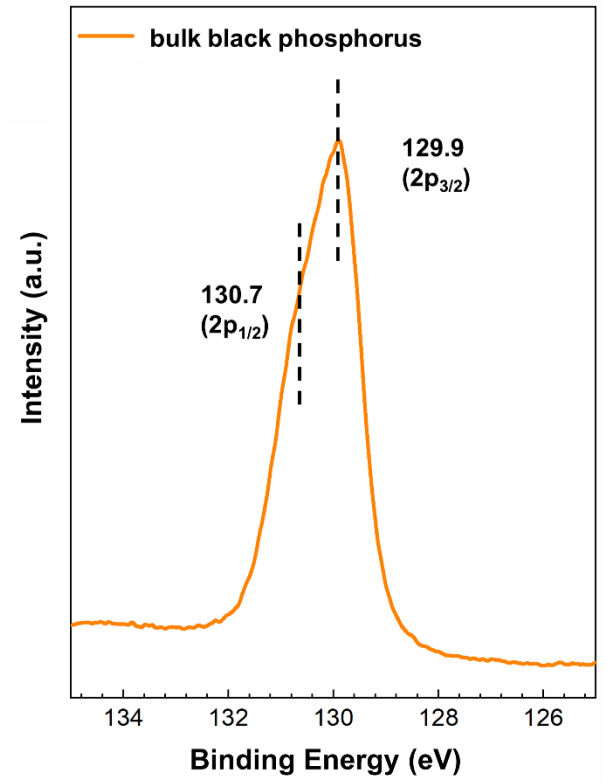

Figure S4. XPS core level spectrum of P 2p for the clean bulk black phosphorus.

Figure S5 displays the simulated STM image based on the atomic model in Figure 4c, which is perfectly matched with the experimental STM image (Figure 4b).

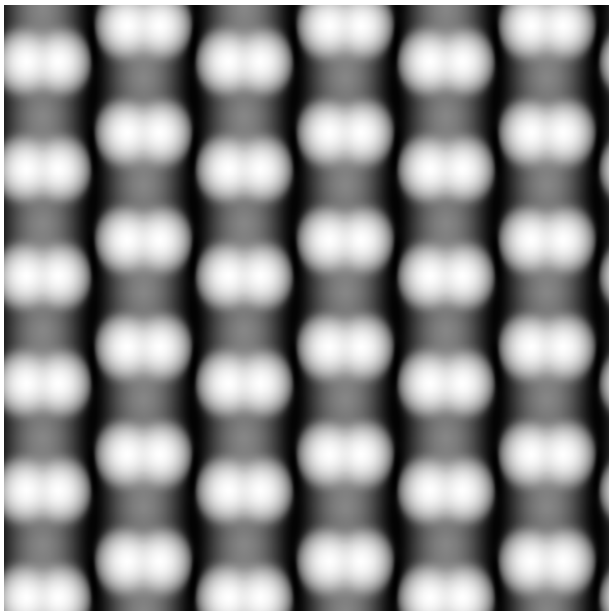

Figure S5. Simulated STM image based on the atomic model in Figure 4c.

Figure S6 displays the STM images of the initial stage, with the ordered P dimers fully covering the substrate.

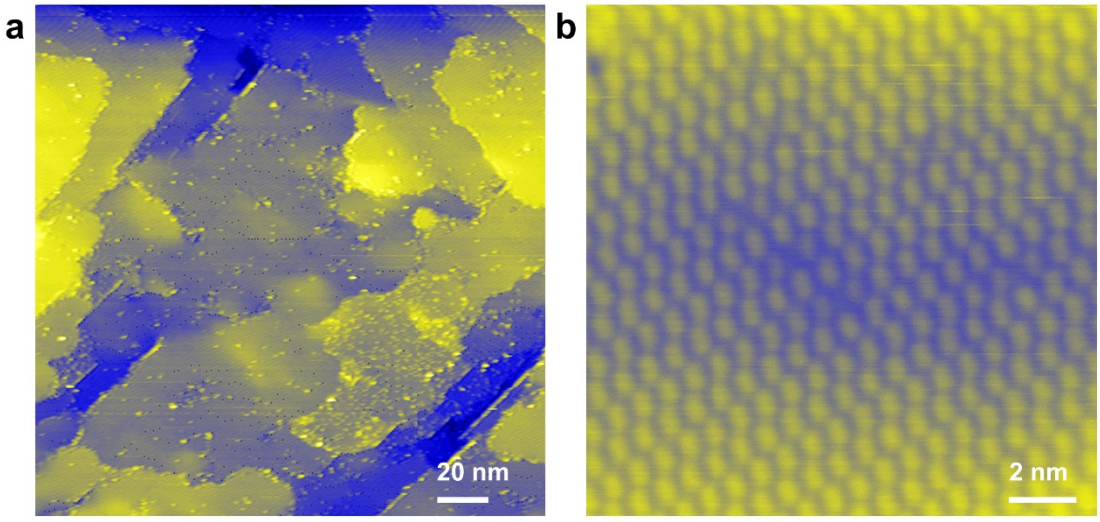

Figure S6. (a) Large-scale and (b) close-up STM images of depositing phosphorus on heated Au(110) (230 °C) for 3 min. (V_s = -1.0 V, 200 × 200 nm^2; V_s = -0.1 V, 15 × 15 nm^2)

Figure S7 is the schematic diagram of the atomistic etching growth mechanism of 1D AuP-chains on Au(110).

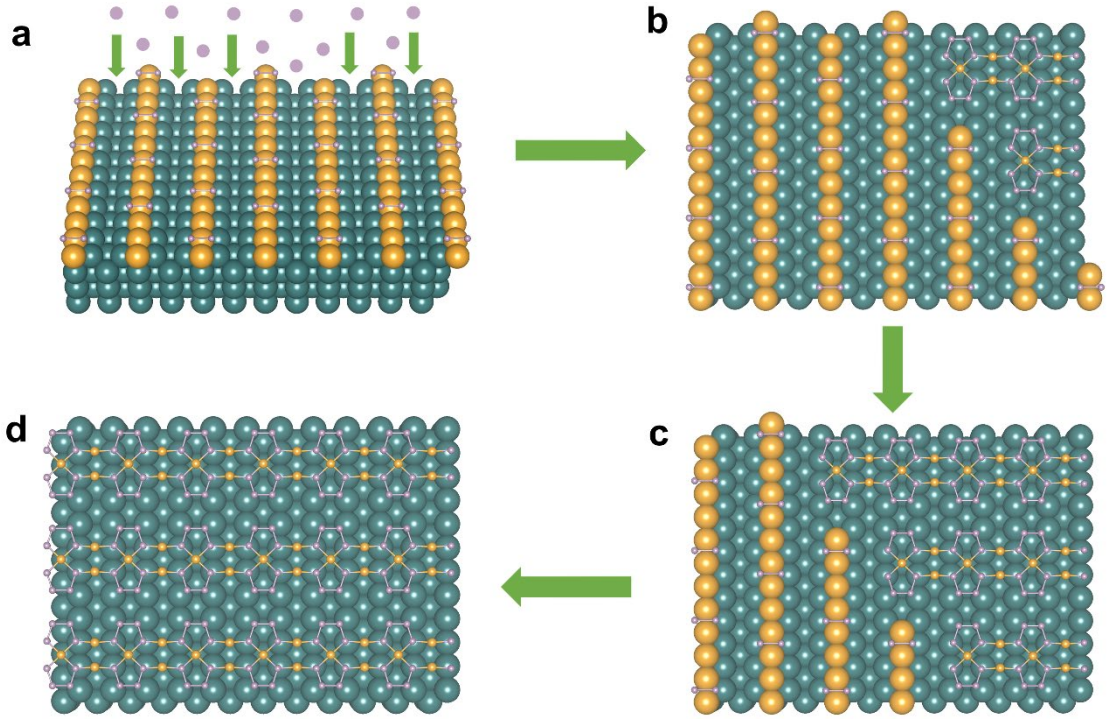

Figure S7. Schematic diagram of the atomistic etching growth mechanism of 1D AuP-chains on Au(110). (a) Deposition of phosphorus atoms and the formation of phosphorus dimers on the reconstructed Au(110) surface. (b) The new-coming P atoms will etch the ordered dimer structure, releasing the Au atoms from the reconstructed surface; then, the released Au atoms will react with the deposited P atoms and coalesce into 1D AuP-chains. (c, d) By the extension of the growth duration, the 1D AuP-chains structure can fully cover the substrate. (purple: P; yellow: surface Au; cyan: bulk Au)

Figure S8 displays the optimized structure of other metal-phosphorus chains by substituting the Au linkers with the metal elements in the same group in the periodic table, e.g. AgP-chains and CuP-chains (Figures S8b and S8c). These metal-phosphorus chains all feature metallic nature, as revealed by the projected density of states in the right panels.

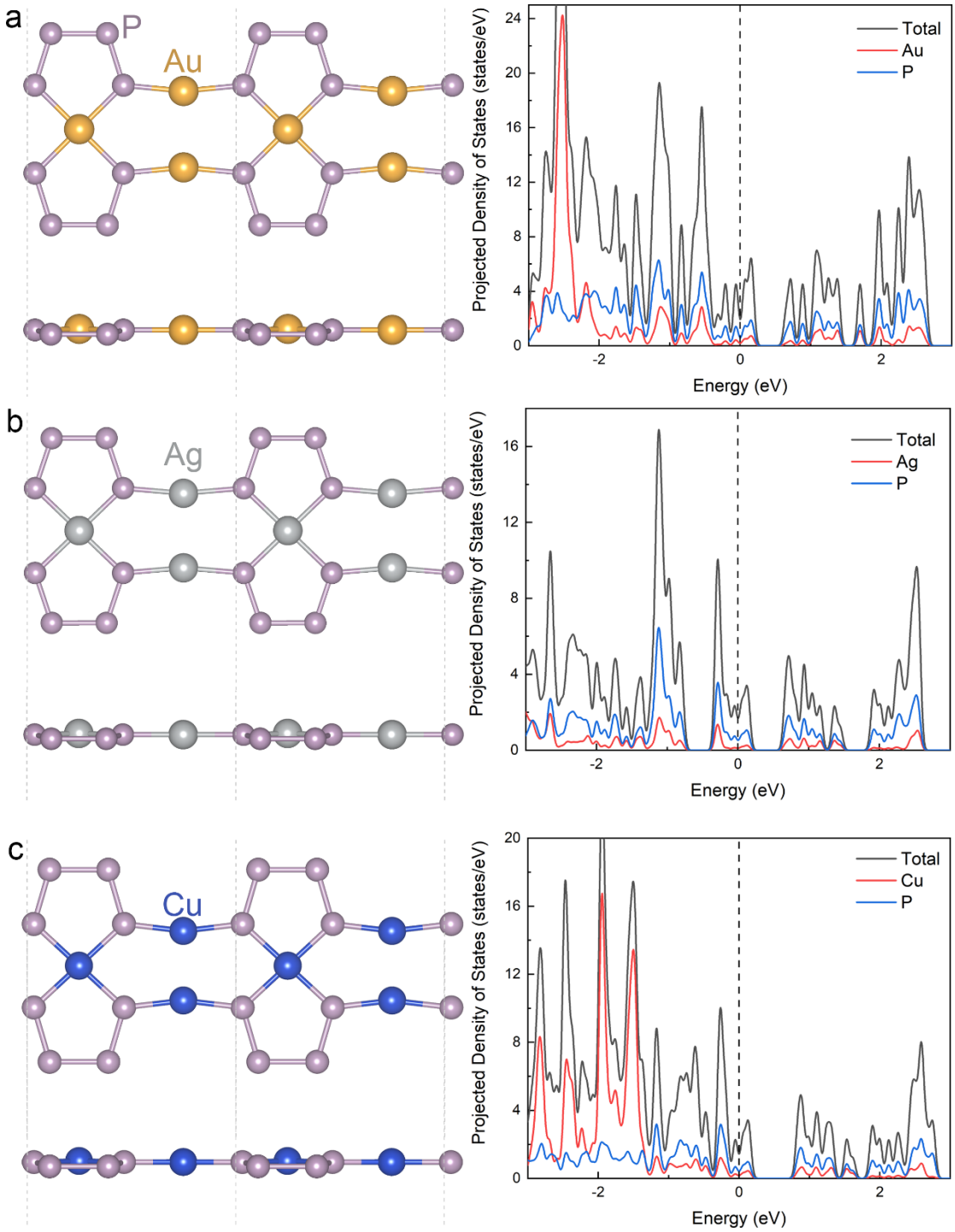

Figure S8. Optimized atomic structures (left panels) and projected density of states (right panels) of free-standing (a) AuP-chain, (b) AgP-chain and (c) CuP-chain. The Fermi level has been set to zero.