Electronic supplementary information for

From Single Atom to Self-Assembled Quantum Single-Atomic Nanowire: Noble Metal Atoms on Black Phosphorene Monolayer

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This file includes:

Supplementary Texts:

S1: The relative stabilities between the two most stable stacking motifs

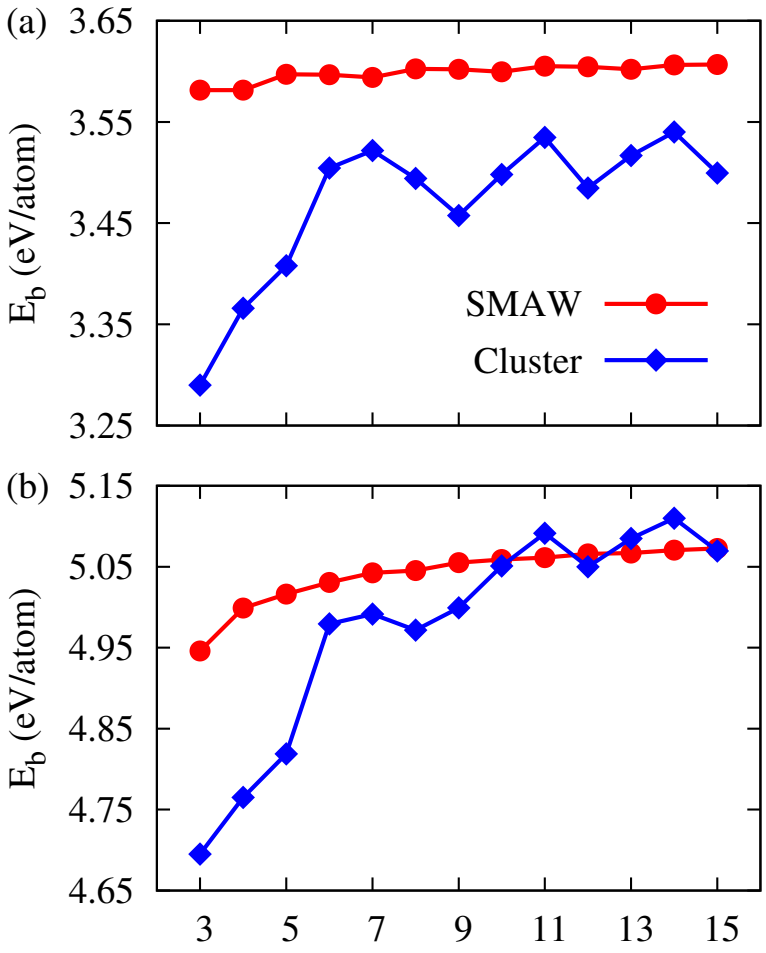

Fig. S1 Average binding energy per atom E_b(n) for (a) Pd_n and (b) Pt_n (n=3-15) between the SMAW and cluster growth models. Here, $E_b(n) = -[E(\mathrm{TM/BP}) - E(\mathrm{BP}) - n \times E(\mathrm{TM_{atom}})]/n)$.

S2: The most stable structures of Pd_n SMAWs (*n*=8-15)

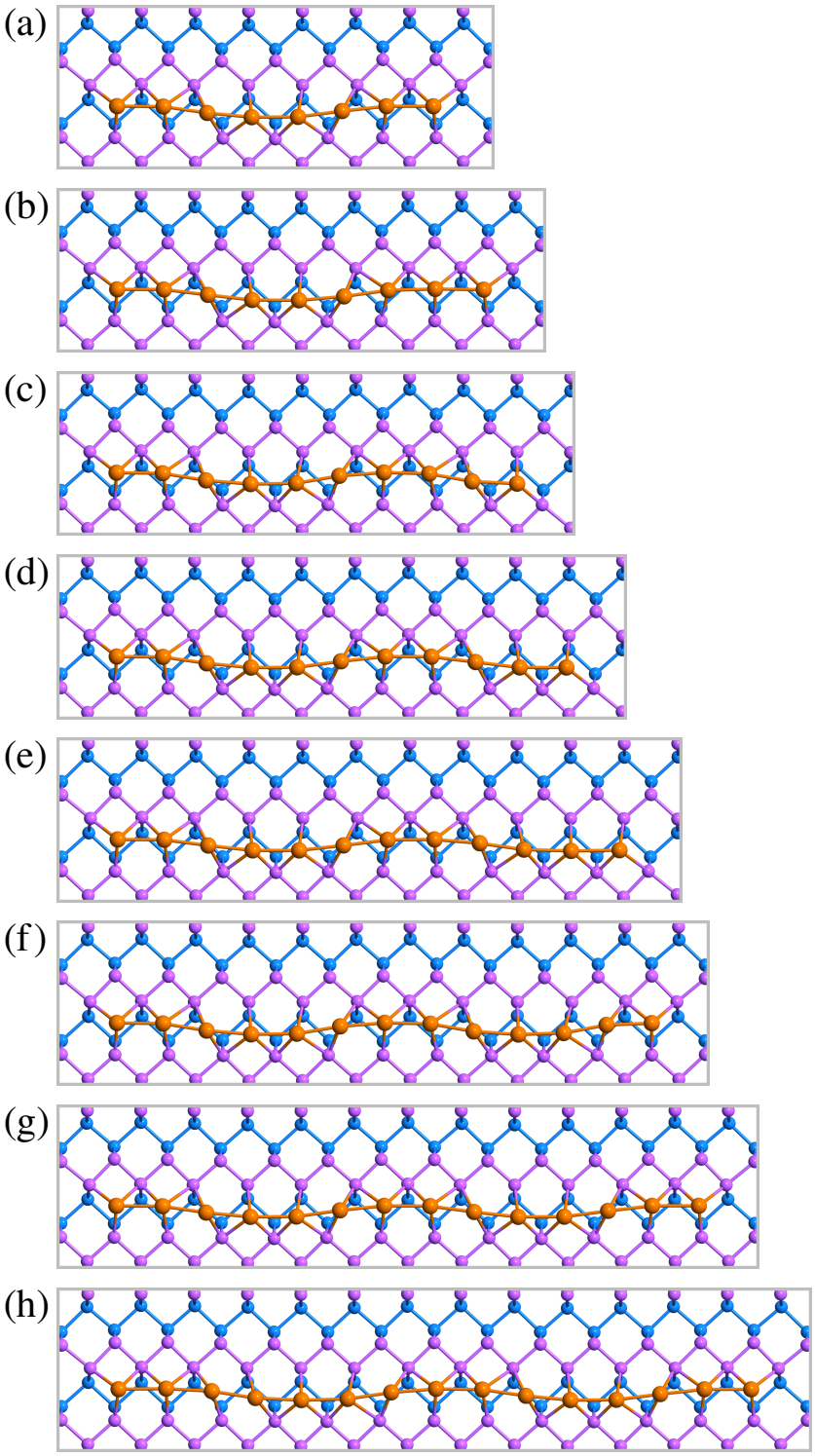

Fig. S2 The most stable structures of Pd_n SMAWs, where (a)-(h) corresponding to n=8-15, respectively.

S3: MD simulations for some representative configurations

The structural stability of the Pd_n and Pt_n SMAWs were examined by MD simulations at room temperature. In Fig. S3, we present the structural snapshots of every 1000 simulation steps (1fs/step) for Pd_8 and Pd_5 SMAWs. One can see that during the whole MD simulation time, the profiles of the Pd_n SMAWs are well-kept, and intriguingly, we observed that the whole SMAWs can slowly drift along the trough of the BP substrates.

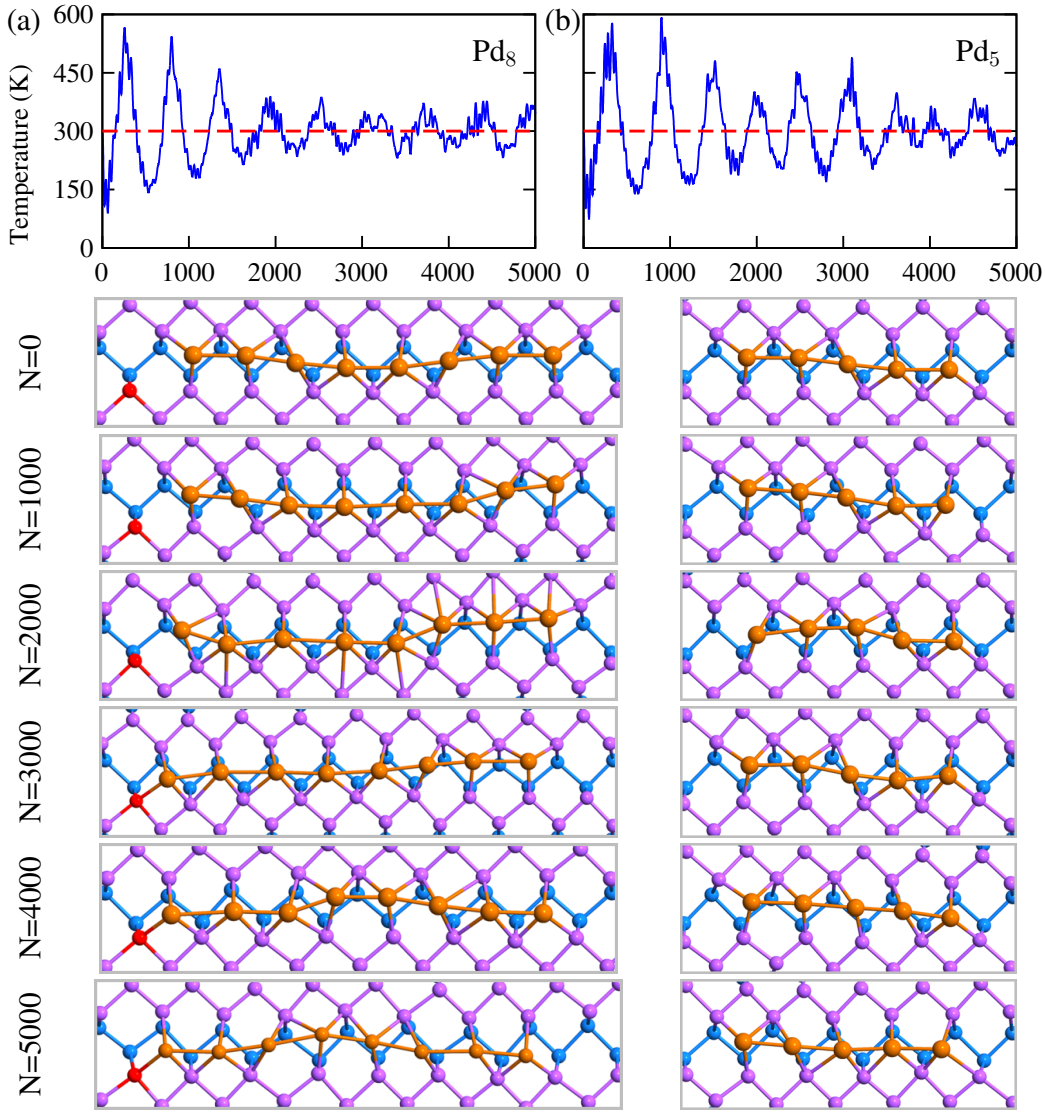

Fig. S3 Molecular Dynamics simulations of (a) Pd_8 and (b) Pd_5 SMAWs. N=0, 1000, ..., 5000 corresponding to the structural snapshot in every 1000 MD steps. One P atom in BP substrate of Pd_8 SMAW was marked to red to locate the Pd_8 atomic chain.

S4: Geometric and electronic structures of the infinite Pd SMAW on BP

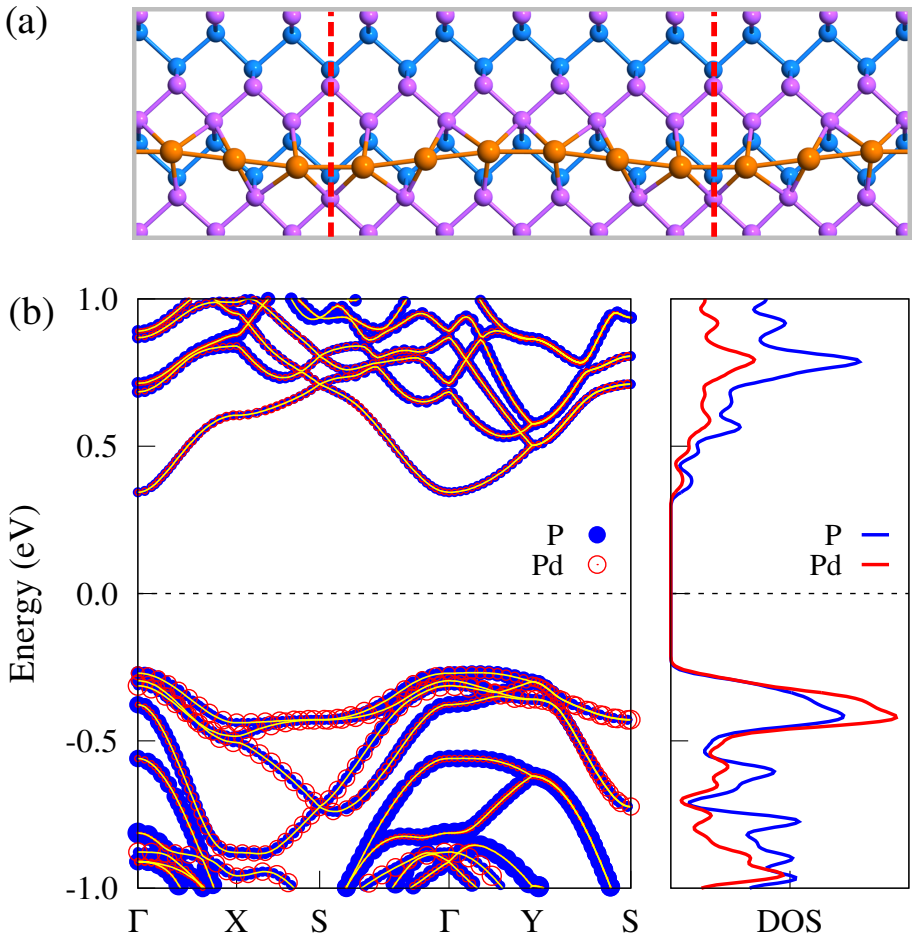

Fig. S4 Geometric and electronic structures of the infinite Pd SMAW on BP. (a) the optimized infinite Pd SMAW on BP with one periodic marked by the red dash line; (b) local projected band structure (left panel) along the high symmetric path and its corresponding density of states (right panel).

S5: The magic characteristics of Pt_n SMAWs

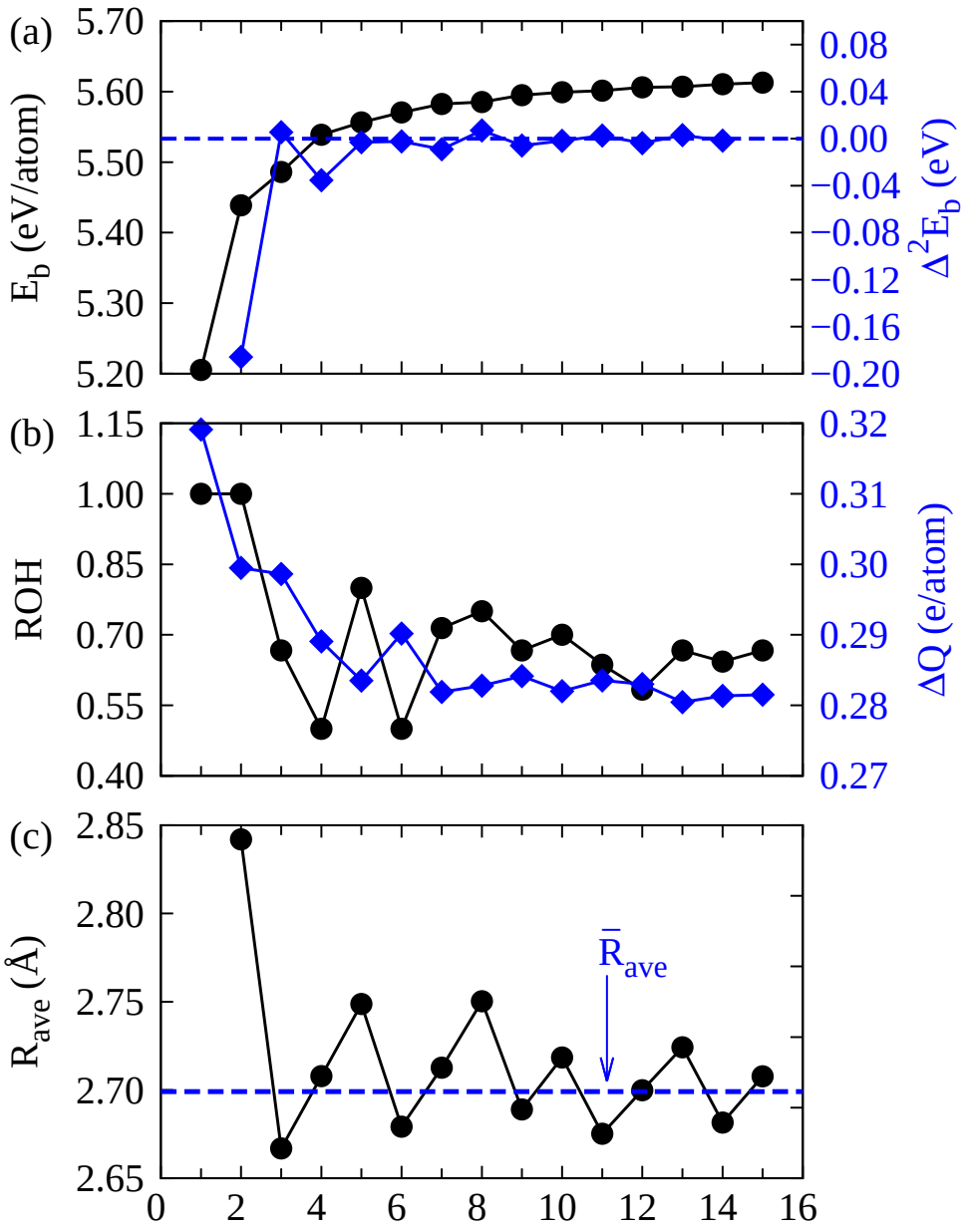

Fig. S5 (a) Average binding energy per atom $E_b(n)$, represented by the black circles; and it's second-order difference represented by the blue diamonds, $\Delta^2 E_b(n)=E_b(n+1)+E_b(n-1)-2E_b(n)$ for Pt SMAWs. (b) The ratio of the hollow sites (ROH, represented by the black circles) on which the Pt atoms in the SMAWs occupy, and the average charge transfer ΔQ (e/atom) from the BP substrate to the Pt SMAWs per Pt atom. (c) Averaged nearest neighboring Pt-Pt bond length.

S6: The semiconducting characteristics of Pd SMAWs

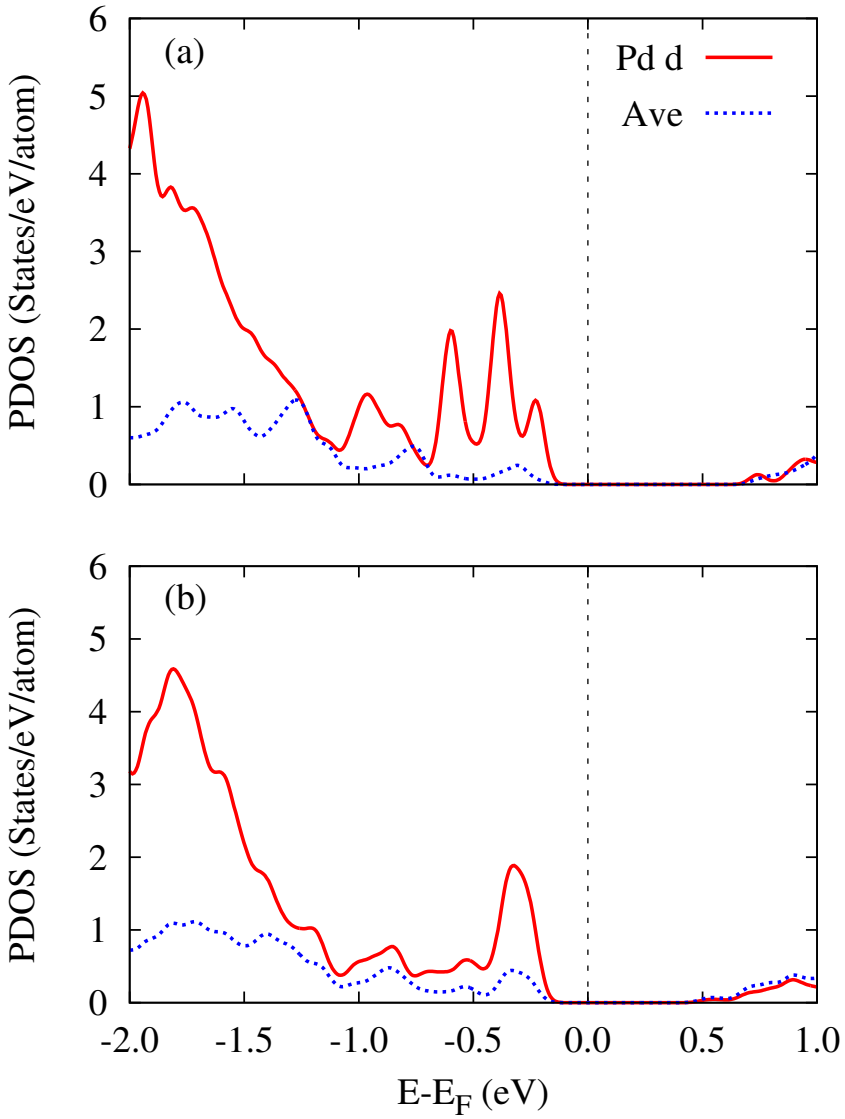

Fig. S6 Local projected density of states (PDOS) of (a) Pd_2/BP and (b) Pd_{15}/BP complexes. Significantly, these Pd_n/BP heterostructures studied in the present work exhibit semiconducting properties with the Pd atoms contributing high DOS by the valence band maximum.