Supporting Information

One-Step Hydrothermal Synthesis of Comb-Like ZnO Nanostructures

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- **S1. EDS of ZnO NSSs**

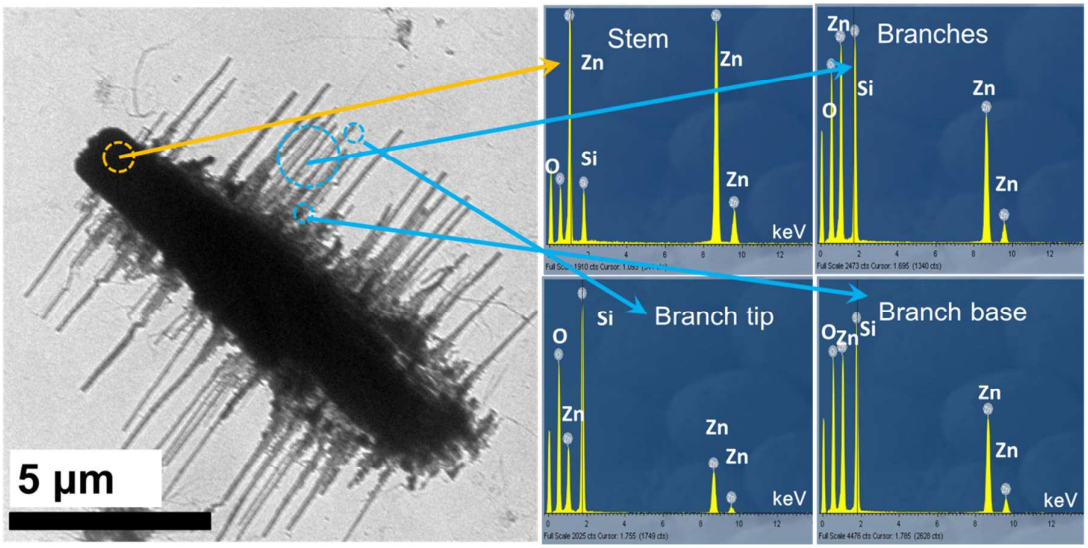

Figure S1: Representative EDS characterizations on the stems and branches of ZnO NSSs show only Zn and O elements exists in ZnO NSSs and Au is not found from typical ZnO NSSs. Si peaks are from the SiO_2 film supported Si_3N_4 TEM grid. The EDS characterization was conducted in TEM.

- **S2. Method of Surface energy calculation**

The surface energies of the related crystalline planes of ZnO were calculated using the Quantum Espresso code[1]. The calculation is based on density functional theory. To study the surface energy, which quantifies the disruption of intermolecular bonds that occurs when a surface is created, a slab with ca. 5–6 ZnO layers was utilized, as illustrated in **Fig. S2** (only Zn-termination surfaces are shown for (0001)). The slab was periodic in the x-y plane with a vacuum layer of 10 Å in the z-direction. The surface energy was obtained from the expression $E_s = (E_{total} - E_{bulk})/2$, where E_{total} is the total energy of the slab, and E_{bulk} is the total energy of bulk ZnO with the same size. The energy difference of E_{total} and E_{bulk} is normalized by 2 due to the two surfaces of the slab. We would like to point out that, currently there is no appropriate way separately to calculate the energy of the polarized Zn- or O-termination surfaces, such as the (0001)[2]. In such a case, we take the average of the surface energy. The surface energies of different crystalline plane of ZnO that are relevant to this research were given in Table 1.

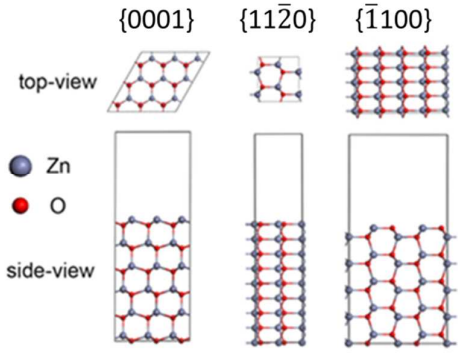

Figure S2: Structural models for surface energy calculations. (Only slabs with Zn-termination surface are shown here.)

References:

[1] http://www.quantum-espresso.org/
[2] A. Wander, F. Schedin, P. Steadman, A. Norris, R. McGrath, T. Turner, G. Thornton, N. Harrison, *Phys. Rev. Lett.* 2001, 86, 3811.

- **S3. The relation between the dimension/distribution of Au nanowires and the morphology of ZnO NSSs.**

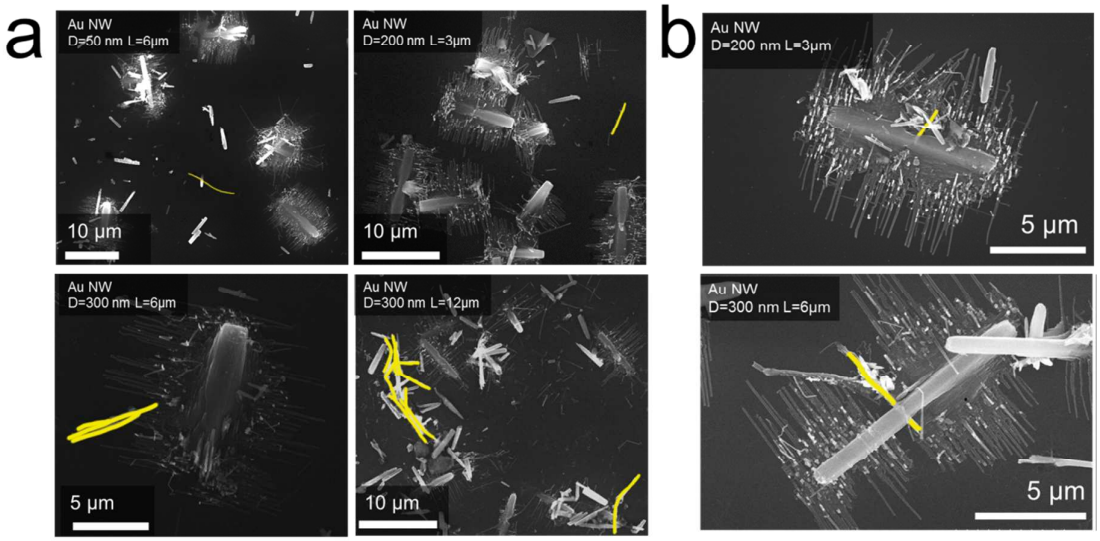

Figure S3: (a) Color enhanced SEM images of ZnO NSSs and the distribution of Au nanowires with different dimensions (Au nanowires are enhanced by yellow color), i.e. D (diameter)=50 nm, L(length)=6μm; D=200 nm, L=3μm; D=300 nm, L=6μm; D=300 nm, L=12μm; (Reaction condition: 10mM $Zn(NO_3)_2{\cdot}6H_2O$, 10mM $C_6H_{12}N_4$, 90°C , 16 hours). (b) Au nanowires transversely inserted in the center of ZnO NSSs.

We studied how the dimension/distribution of Au nanowires can determine growth of ZnO NSSs: Au nanowires with different dimensions (i.e. diameter 50nm, 200nm and 300nm and Length from 3μm to 12μm) were dispersed on individual silicon wafers and reacted in a solution of 10mM $Zn(NO_3)_2{\cdot}6H_2O$ and 10mM $C_6H_{12}N_4$ at 90°C for 16 hours. When the reaction was accomplished, we gently took out the sample, without further washing, dried in air, and characterized with Scanning Electron Microscopy (SEM). We observed very small amount (<5%) of Au nanowires were embedded in ZnO NSSs, most of which transversely inserted through the middle of ZnO stems as shown in Fig. S3(b). Overall, there is no direct correlation between the distribution (location, orientation, shape) of the Au nanowires and ZnO NSSs for majority ZnO NSSs. Representative color-enhanced SEM images are shown in Fig. S3(a). Furthermore, we didn't find significant morphology variation among ZnO NSSs catalyzed by Au nanowires of different dimensions. An exception is that 10 nm Au nanoparticles can assist vertical growth of ZnO nanorods as discussed in the main text.