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Supporting Information

Catalytic asymmetric hydrogenation reaction by *in situ* formed ultra-fine metal nanoparticles in live thermophilic hydrogen-producing bacteria

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Scheme S1. Illustration of hydrogen-producing bacteria supported PdNPs composites for asymmetric C=C hydrogenation of diacetone alcohol to (R)-2-methyl-2,4-pentanediol.



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Figure S1. The digital photograph showed the color change of the obtained suspensions, indicating the formation of B-AuNPs and B-PdNPs nanohybrids.



Figure S2. (A) XPS analysis surveys of B-AuNPs; (B) Wide-angle powder XRD pattern of B-AuNPs nanocomposites. The wide-angle X-ray diffraction pattern exhibits five peaks, which could be indexed as the (111), (200), (220), (311) and (222) reflections of the face centered cubic structure of crystalline Au⁰.



Figure S3. (A) XPS analysis surveys of B-PdNPs; (B) Wide-angle powder XRD pattern of B-PdNPs nanocomposites. The wide-angle X-ray diffraction pattern exhibits five peaks, which could be indexed as the (111), (200), (220), (311) and (222) reflections of the face centered cubic structure of crystalline Pd⁰.



Figure S4. The hydrogen-producing ability of B-AuNPs.



Figure S5. UV–vis spectra of aqueous solutions of *o*-nitroaniline and H₂ in the presence of AuNPs (13 nm) measured at different time intervals as control experiment.

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Figure S6. Fluorescence microscopic visualization of pristine bacteria (A, B) and B-AuNPs composites (C, D). Fluorescence microscopic visualization of adherent bacteria after adoption of the different live/dead stainings: FDA/PI. Under fluorescence microscopy, green and red stains indicate viable and dead cells, respectively, scale bar = 10 μm.



Figure S7. Fluorescence microscopic visualization of pristine bacteria (A, B) and B-PdNPs composites (C, D). Fluorescence microscopic visualization of adherent bacteria after adoption of the different live/dead staining: FDA/PI. Under fluorescence microscopy, green and red stains indicate viable and dead cells, respectively, scale bar = 10 μm.

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Figure S8. TEM of (A) B-AuNPs and (B) B-PdNPs after catalytic process.