## **Electronic Supplementary Information (ESI) for**

## Megranate-Like Nanoreactor with Multiple Cores and an Acidic Mesoporous Shell for a Cascade Reaction

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State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun 130012, People's Republic of China. E-mail: huoqisheng@jlu.edu.cn; Fax: +86-431-85168624; Tel: +86-431-85168602 **Synthesis of silica nanorattles-SH:** Silica nanorattles-SH were prepared according to literatures with some minor modifications. In a typical reaction, solution A (2 mL of TEOS in 18 mL of ethanol), solution B (20 mL of 28 wt % aqueous NH<sub>3</sub> and 60 mL of ethanol) and solution C (100  $\mu$ L of TSD in 8 mL of ethanol) were prepared. Solution A (5 mL) was added dropwise into solution B and reacted for 10min under vigorously stirring to form the cores. Then, solution C and identical volume of solution A were added into the reaction mixture synchronously at a rate of 1 mL/min, to form the middle layer of organicsilica framework. Lastly, remaining solution A and MPTMS (60  $\mu$ L) were added to form the outer layer of silica shell. The reaction was kept for 3 hours at 30 °C. The hybrid silica spheres were isolated by centrifugation and washed with ethanol and water repeatedly and lastly resuspended in water. Silica nanorattles-SH were produced by etching the as-prepared hybrid silica spheres with 10 wt % HF (aqueous solution). Briefly, a certain amount of 10 wt % HF was added dropwise into silica nanorattles-SH suspension, stirring for 10 min. The product was sufficiently washed repeatedly with water.

Synthesis of silica nanorattles-SO<sub>3</sub>H: Silica nanorattles-SO<sub>3</sub>H were prepared according to literatures with some minor modifications. The silica nanorattles-SH (1.0 g) were dispersed in  $H_2O_2$  (40 g, 30 wt %) and stirred at RT for 24 h before centrifugation. The dried silica nanorattles-SO<sub>3</sub>H (1.0 g) were then stirred in HCl (200 mL, 0.01 M) for 12 h at RT for acidification. After being thoroughly washed with deionized water, the solid product was dried at 60 °C overnight.



Fig. S1 Pore size distribution obtained from the BJH model applied to the adsorption branch of silica nanorattles-SH



Fig. S2 Pd 3d XPS spectra of megranate-like of Pd-silica nanorattles-SO<sub>3</sub>H



Fig. S3 a, b) TEM images, and c, d, e, f,) HRTEM images of (a, c, e) Pt-silica nanorattles-SH; (b, d, f) Au-silica nanorattles-S



Fig. S4 Elemental mappings of Pt-silica nanorattles-SH



Fig. S5 Elemental mappings of Au-silica nanorattles-SH



**Fig. S6** Schematic illustration the megranate-like Pd-silica nanorattles-SO<sub>3</sub>H as a nanoreactor for the cascade reaction

## Characterization data for 2-(2-nitrophenyl)-1H-benzimidazole

<sup>1</sup>H-NMR (300 MHz, (CD<sub>3</sub>)<sub>2</sub>SO):  $\delta$  8.42 (s, 4H), 7.67 (s, 2H), 7.28 (m, 2H), 3.33 (s, 1H). HRMS ESI: [M+H]<sup>+</sup>, for [C<sub>13</sub>H<sub>9</sub>N<sub>3</sub>O<sub>2</sub>+H]<sup>+</sup> calcd. 240.1; found 240.2.