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Supplementary Information

Structural rearrangements of Ru nanoparticles supported on carbon nanotubes under microwave irradiation

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Experimental Section

Ruthenium nanoparticles supported on carbon nanotubes (Ru/CNTs) were synthesized by a microwave thermolysis method. $Ru_3(CO)_{12}$ was mixed together with CNTs and grinded for 20 minutes. Argon was flowed on the mixture for 2 hours at a flow rate of 100 mL/min, followed by microwave treatment at a quartz-tube reactor with a frequency of 2.45 GHz (the power is 800 W) as the radiation source for 1, 3, and 5 min. Samples were then taken out after cooling to room temperature. The loading content of Ru is 5.0 wt%. They were named as Ru/CNTs-1min, Ru/CNTs-3min, and Ru/CNTs-5min, respectively.

X-ray diffraction (XRD) analysis of the CNTs and Ru/CNTs samples were carried out using a Rigaku D/Max-RB diffractometer with Cu K_α monochromatized radiation

source (λ=1.54178 Å) and a D8 Advance theta/theta diffractometer (Bruker AXS) with Cu $K_{\alpha 1+2}$ radiation (λ=1.54186 Å), respectively. A FEI Cs-corrected Titan 80-300 microscope operated at 300 kV was employed to conduct structural investigations of Ru/CNTs samples by using TEM, HRTEM, and STEM modes. HRTEM simulation was performed by using JEMS software and a supercell approach for the single crystal Ru nanoparticle (copyright P. A. Stadelmann, EPFL, Switzerland). The simulations of particle shapes were conducted by combing Atom software and HRTEM simulation. The Ru/CNT samples were ultrasonically dispersed in ethanol, and then a drop of the solution was deposited on a holey C/Cu TEM grid to be used for HRTEM and high-angle annular dark-field (HAADF)-STEM characterization.

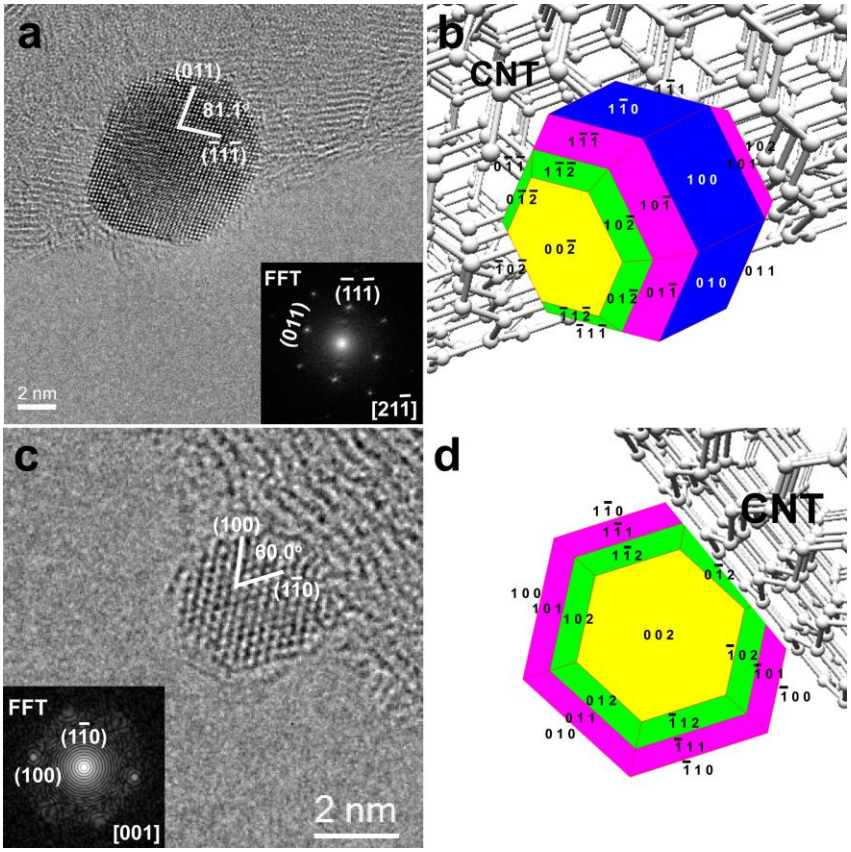

Fig. S1 HRTEM images of Ru/CNTs-5min sample (a, c) together with corresponding shapes with faceting configurations (b, d). Insets in Figs. S1a and S1c are the local FFT of the HRTEM images.

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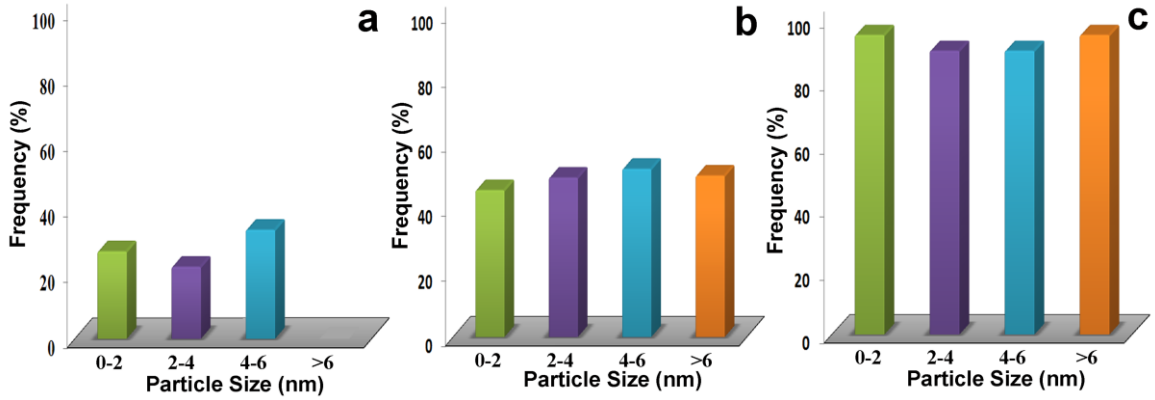

Fig. S2 The frequency of single crystal Ru nanoparticles against particle size for Ru/CNTs-1min (a), Ru/CNTs-3min (b), and Ru/CNTs-5min (c) samples.

Table S1 Measurement of central tendency (particle number, mean, median, and standard deviation) for Ru/CNTs-1min, Ru/CNTs-3min, and Ru/CNTs-5min samples by using STEM images.

Sample	Particle number	Mean (nm)	Median (nm)	Standard deviation
Ru/CNTs-1min	673	1.8	2.2	0.8
Ru/CNTs-3min	683	2.3	2.3	1.1
Ru/CNTs-5min	675	2.6	2.3	1.5