Supporting information

Ruthenium Nanoparticle-Decorated Porous Organic Network for Direct Hydrodeoxygenation of Long-Chain Fatty Acids to Alkanes

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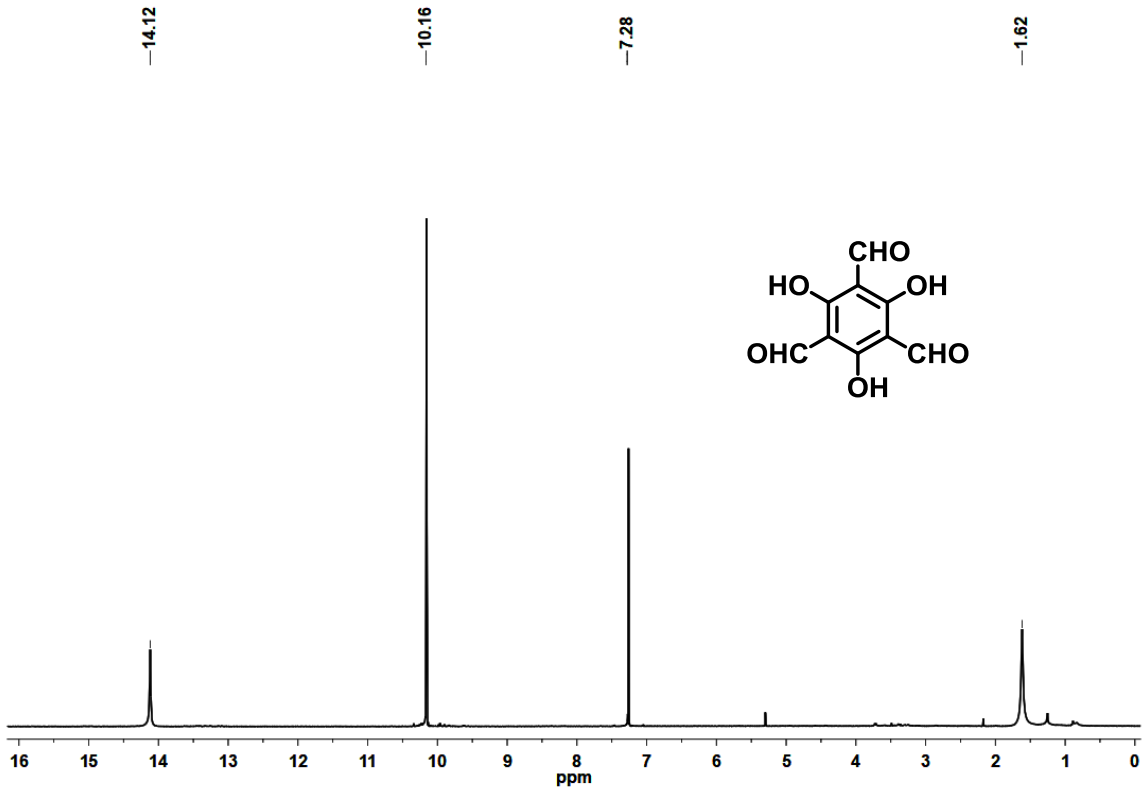

Fig. S1 ^{1}H NMR Spectrum of 1,3,5-triformylphloroglucinol (Tp).

1,3,5-triformylphloroglucinol: ^{1}H NMR (400 MHz, $CDCl_3$) δ 14.12 (s, 3H); 10.16 (s, 3H).

Computational Methodology

Quantum chemical calculations were performed using the density functional theory (DFT) method to analyze the molecular and electronic structure including the electrostatic potential (ESP) of a polymer model system in vacuo. The B3LYP[2, 3] functional in conjunction with the 6-31G* basis set[4, 5] was used for geometry optimizations and generation of the ESP. The CHelpG scheme[6] was used to select points for charge fitting of the ESP. All calculations were performed using Gaussian 09 Revision E.01.[7] We created a ring-shaped molecular model structure from the periodic structure for DFT calculations by cutting and hydrogen termination of the molecular model as shown in Fig. S2. We performed geometry optimization for this model system and used its optimized structure for generation of the ESP.

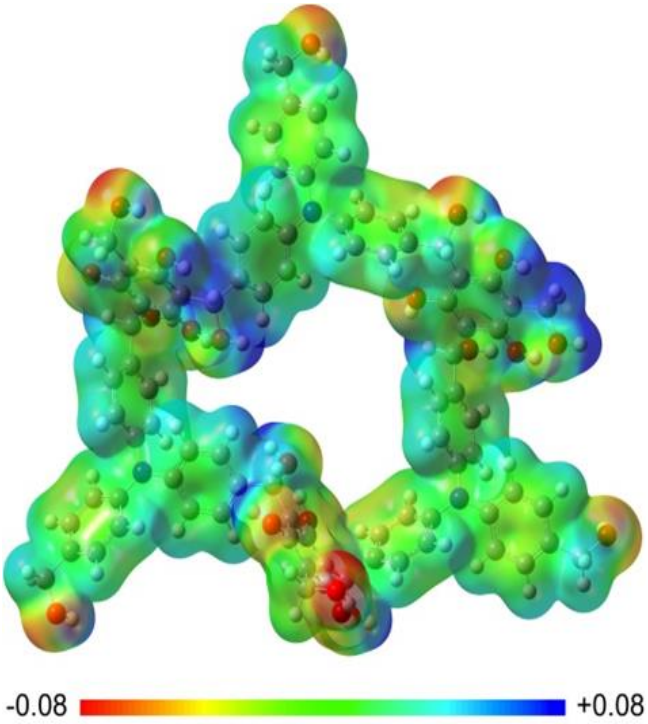

Fig. S2 The ESP (in a.u., see the colored bar for the explanation of the color code) mapped onto the electron density (iso value = 0.004 a.u.) of the molecular models.

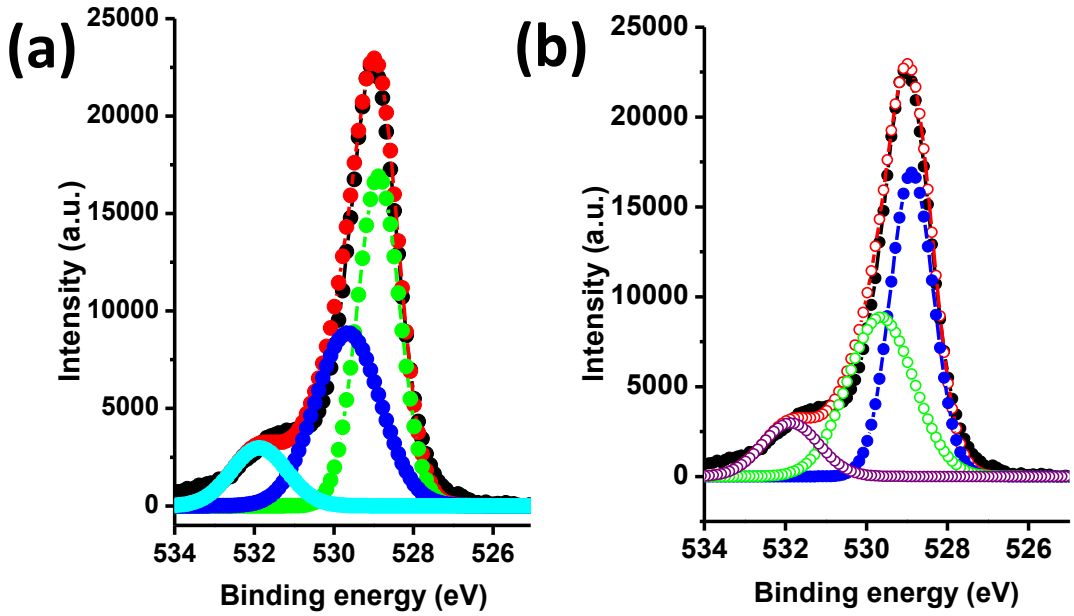

Fig. S3 XPS survey spectra: O 1s region of TpPON (a) and Ru@TpPON (b) materials respectively.

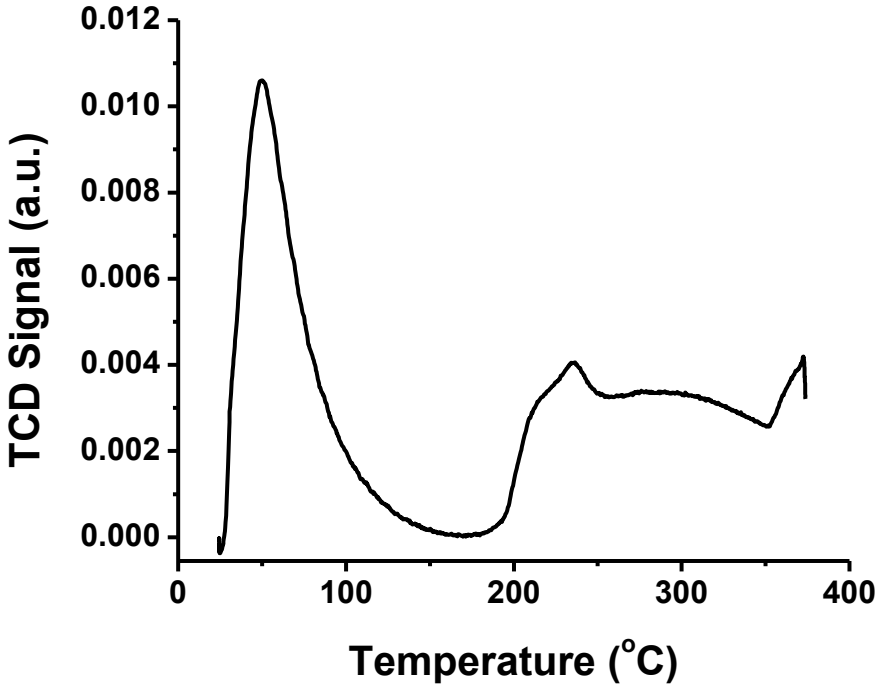

Fig. S4 NH_3-TPD profile of Ru@TpPON.

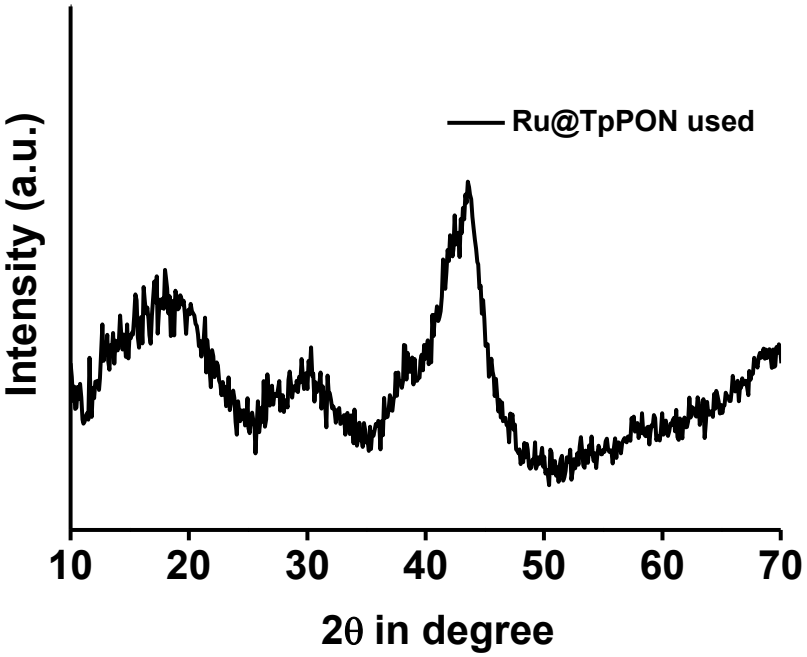

Fig. S5. Powder diffraction patterns of used Ru@TpPON catalyst.

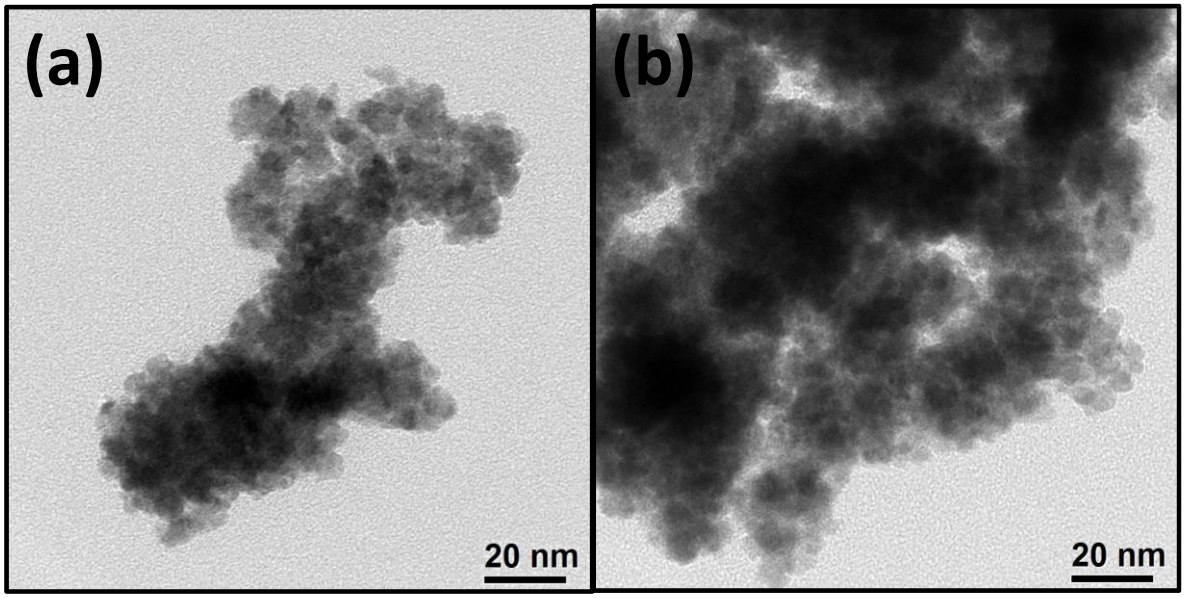

Fig. S6 HR-TEM images of used Ru@TpPON catalyst.

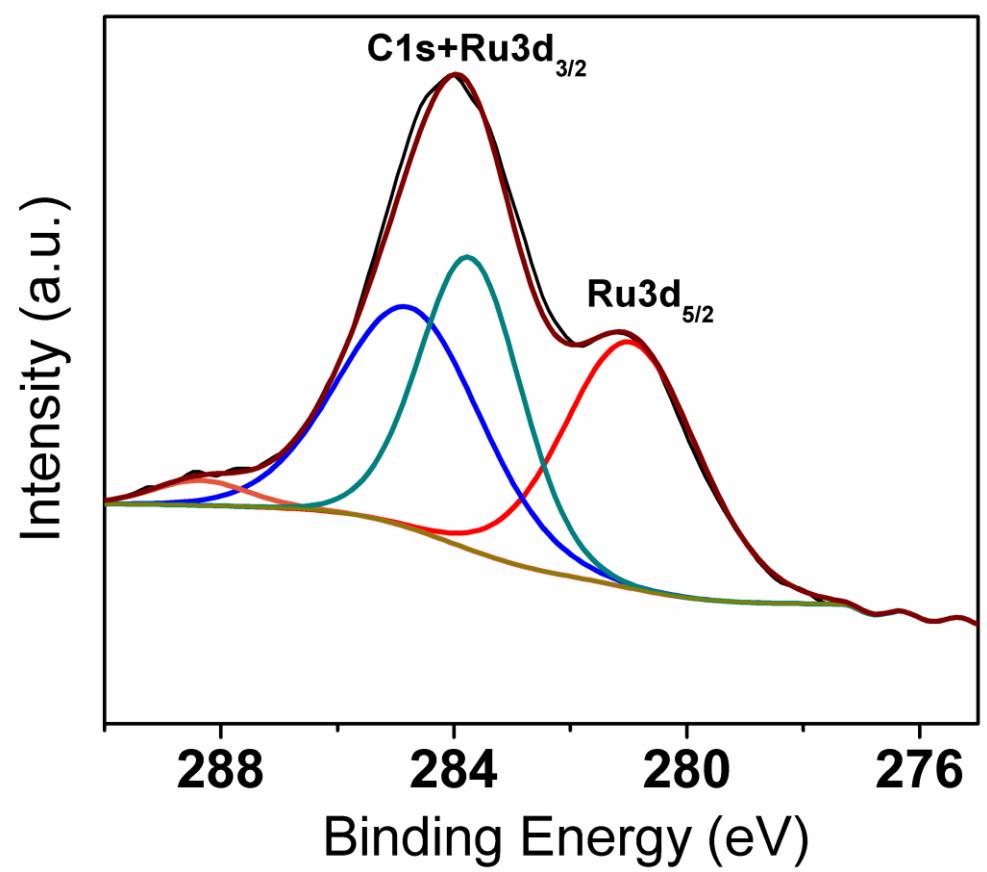

Fig. S7 XPS spectrum in Ru-3d region of used Ru@TpPON catalyst.

References

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