Supplementary Materials

On-surface synthesized magnetic nanoclusters of ferrocene derivatives

Makoto Sakurai*

International Center of Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science (NIMS), Tsukuba 305-0044, Japan.

*Correspondence to: Dr. Makoto Sakurai, International Center of Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba 305-0044, Japan. E-mail: sakurai.makoto@nims.go.jp

Estimation of magnetization of the molecule

The magnetic states of the Fe ions within the C₂₄H₂₄FeNP nanoclusters were investigated by calculating the magnetization of the molecule as follows. The magnetization $M_{FD}(T)$ of the ferrocene derivative can be expressed in terms of the total magnetization $M_{tot}(T)$ of the GO nanosheet reacted with ferrocene derivatives and the magnetization $M_{GO}(T)$ of the pristine GO sheet:

$$M_{\text{tot}}(T) = \frac{W_{\text{GO}}}{W_{\text{GO}} + W_{\text{FD}} \times N_{\text{NC}} \times D_{\text{NC}}} M_{\text{GO}}(T) + \frac{W_{\text{FD}} \times N_{\text{NC}} \times D_{\text{NC}}}{W_{\text{GO}} + W_{\text{FD}} \times N_{\text{NC}} \times D_{\text{NC}}} M_{\text{FD}}(T)$$
(1)

Here, W_{GO} is the mass of the pristine GO nanosheet per unit area, W_{FD} is the mass of a single molecule. N_{NC} is the number of the molecules in the nanocluster; it was estimated from the average height and diameter of the nanocluster and the lateral intermolecular distance, and by assuming height (see Figure 3G) to be 0.22 nm, i.e., 10 % longer than that in AFc-GO sheets ^[16]. D_{NC} is the number density of nanoclusters on the GO nanosheet, and it was experimentally determined by counting the nanoclusters in the TEM images.



Supplementary Figure 1. Right panels show the energy dispersive X-ray spectroscopy (EDX) spectra of white area (nanocluster site) and dark area (GO nanosheet site) marked in the transmission electron microscope (TEM) image.



Supplementary Figure 2. Histogram of (a) diameter and (b) height of $C_{24}H_{24}FeNP$ nanoclusters on GO nanosheet (reaction time: 46 h). Red solid lines show Gaussian fit of the data.