An experimental and theoretical study on the scanning tunneling spectroscopy of europium nanowires encapsulated in carbon nanotubes

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Metal nanowires, whose diameter is typically one to several atoms, are one of the most ideal one-dimensional nanosystems, the preparation and characterization of these have been difficult because of their high reactivity towards air. Previously, we have found that ultrathin europium (Eu) nanowires can be synthesized in the interior space of carbon nanotubes (CNTs).[1-2] Here, the spatially-resolved electronic structure of a CNT encapsulating the Eu nanowire (EuNW@CNT) investigated with scanning tunneling spectroscopy (STS) reveal that an electronic state, which is absent in the corresponding pristine CNT, appears just below the first van-Hove singularity of the CNT. To identify the origin of this electronic state, we have calculated the electronic states of EuNW@CNTs by density functional theory using the generalized gradient approximation + U method.

Figure 1(a) presents a geometrically optimized structure of EuNW@CNT which is shown schematically along the tube axis. As shown in the figure, two rows of Eu atoms align at the middle of the interior space of the CNT. Atom- and spin-resolved density of states (DOS) shown in Fig. 1(b) clearly demonstrate that a peak arising from Eu-6s state exists at the gap region of CNT. The C-2p state also has a finite DOS at the energy where the Eu-6s state exists. This suggests that the Eu encapsulation can generate an additional peak in the STS spectra, which is consistent with the current observation.

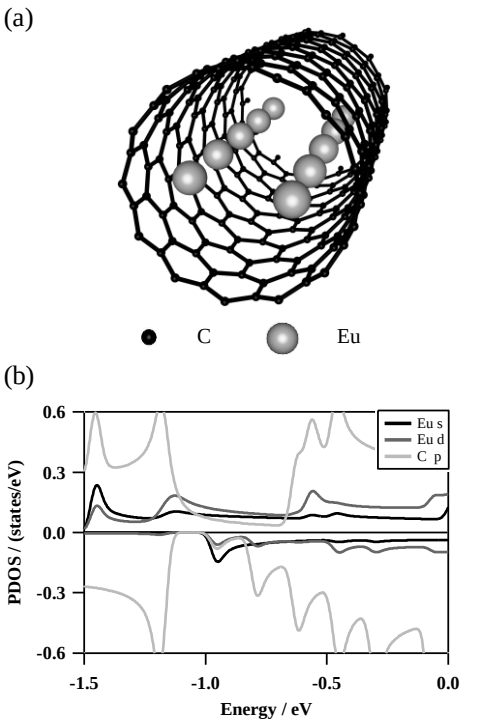

Fig. 1(a) Structure model of EuNW@CNTs. (b)Partial DOS. +y axis shows spin up states and –y spin down states.

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[2] R.Nakanisihi *et al*. Phys. Rev. B **86**, 115445, (2012).

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