Supporting Information

Structural, Electronic and Transport Properties of Gd/Eu Atomic Chains Encapsulated in Single-walled Carbon Nanotubes

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Figure S1. Binding energy per Gd atom of ferromagnetic (FM) and anti-ferromagnetic (AFM) off-centered single-atom Gd chains encapsulated in (8,0) SWCNT as a function of plane-wave cutoff energy using 2 k-points.
Figure S2. Binding energy per Gd atom of ferromagnetic off-centered single-atom Gd chains encapsulated in (8,0) SWCNT as a function of the number of $k$-points using 220 eV plane-wave cutoff energy.