Electronic Supplementary Material (ESI) for Nanoscale
This journal is © The Royal Society of Chemistry 2012

Redox-switchable devices based on functionalized graphene nanoribbons

Daniele Selli, Matteo Baldoni, Antonio Sgamellotti and Francesco Mercuri*

CNR-ISTM, UdR INSTM and Department of Chemistry, University of Perugia, via Elce di Sotto 8, 06123 Perugia, Italy.

SUPPORTING INFORMATION

This journal is © The Royal Society of Chemistry 2012

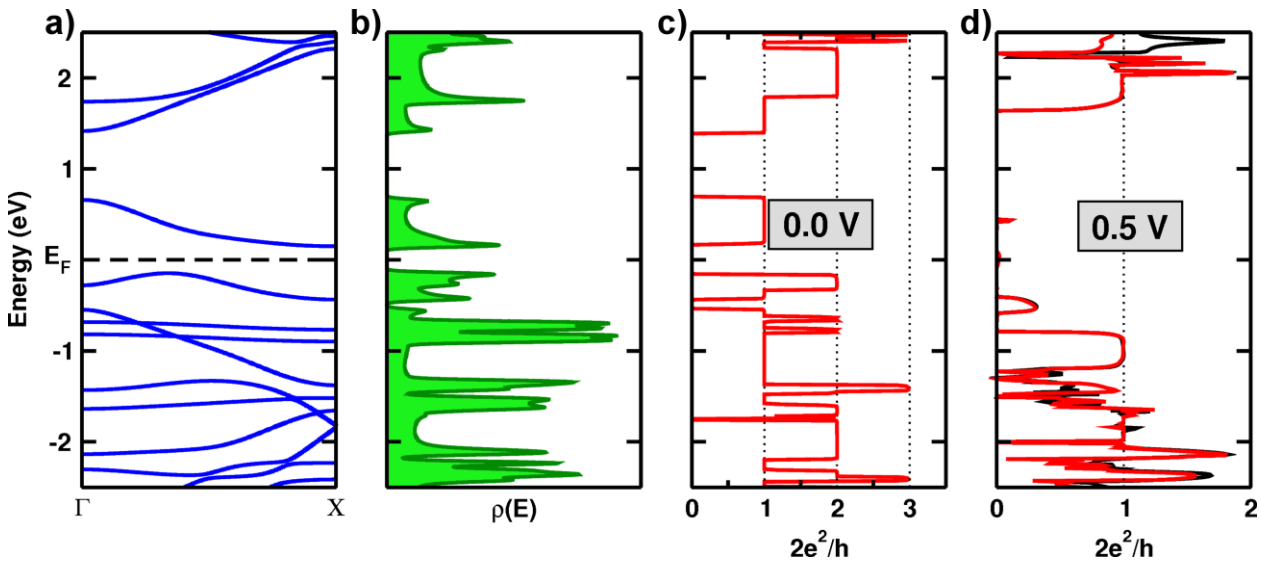

Fig. S1. Band structure, DOS and transmission spectra at no bias and at a bias of +0.5V of species **4** (see text) in the spin-polarized state.

This journal is © The Royal Society of Chemistry 2012

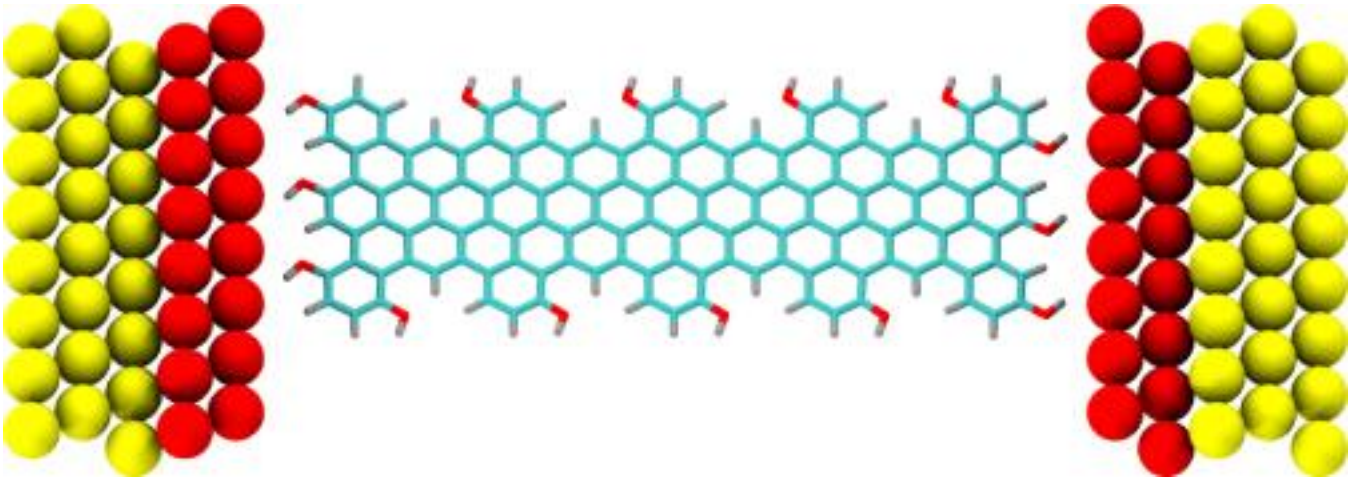

Fig. S2. Set-up for the redox system **3**/**4** (here shown in the reduced state) embedded between two gold electrodes. Gold atoms included in the scattering region are highlighted in red. The distance between the GNR and the gold surface was optimized at the DFT level.

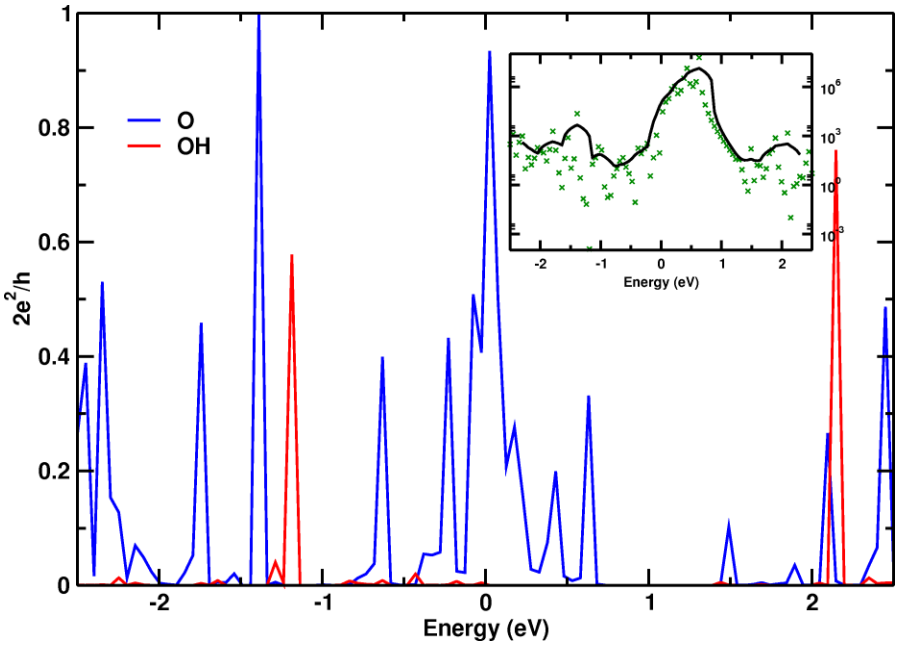

Fig. S3. Transmission spectra of system **3** (blue curve) and **4** (red curve) between gold electrodes (see Figure S2). Inset: ratio between the two transmission spectra.

This journal is © The Royal Society of Chemistry 2012

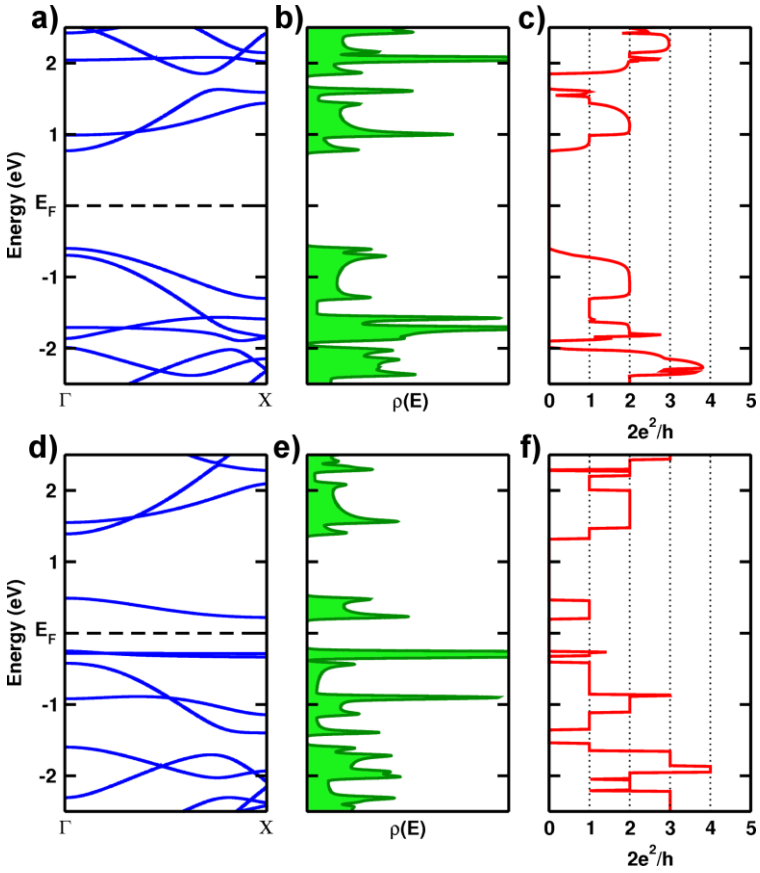

Fig. S4. Band structure, DOS and transmission spectra of species **5** and **6** in Figure 6a-b (see text).

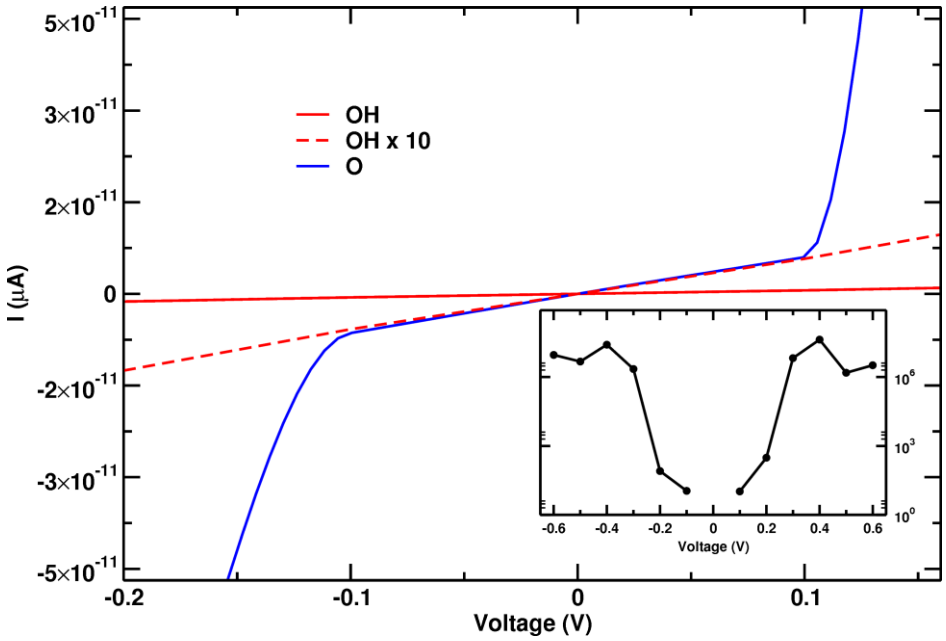

Fig. S5. I(V) characteristics of the switch in Figure 6a-b in the reduced (**5**, continuous red curve) and oxidized (**6**, blue curve) states. A magnification of the values for the reduced state (dashed red curve) by a factor 10 is also shown for clarity. Inset: ON/OFF ratio (logarithmic scale).

This journal is © The Royal Society of Chemistry 2012

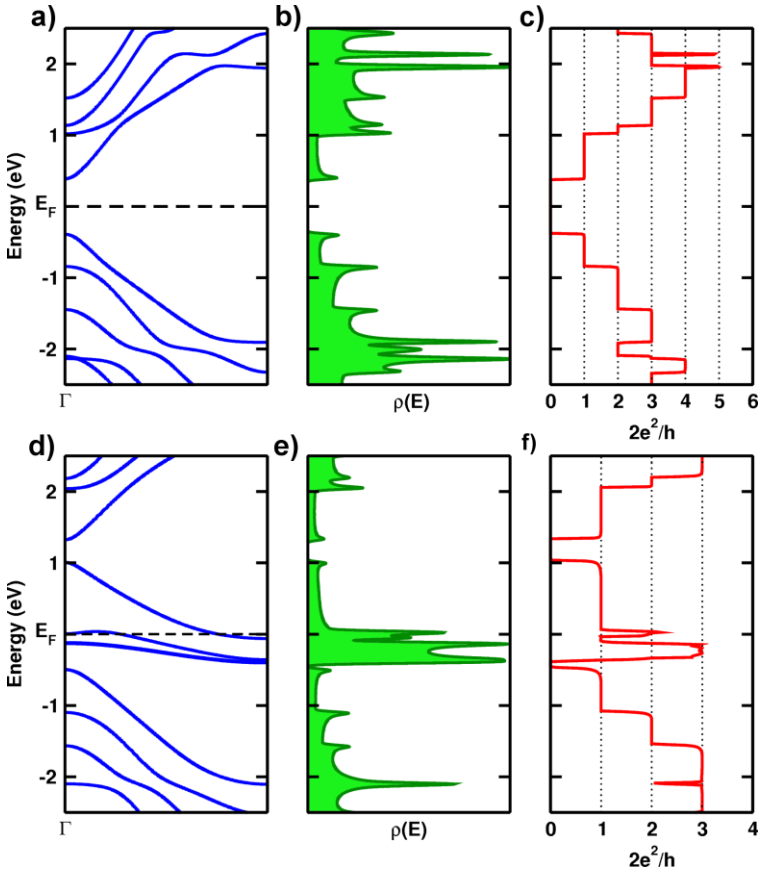

Fig. S6. Band structure, DOS and transmission spectra of species **7** and **8** in Figure 6c-d (see text).

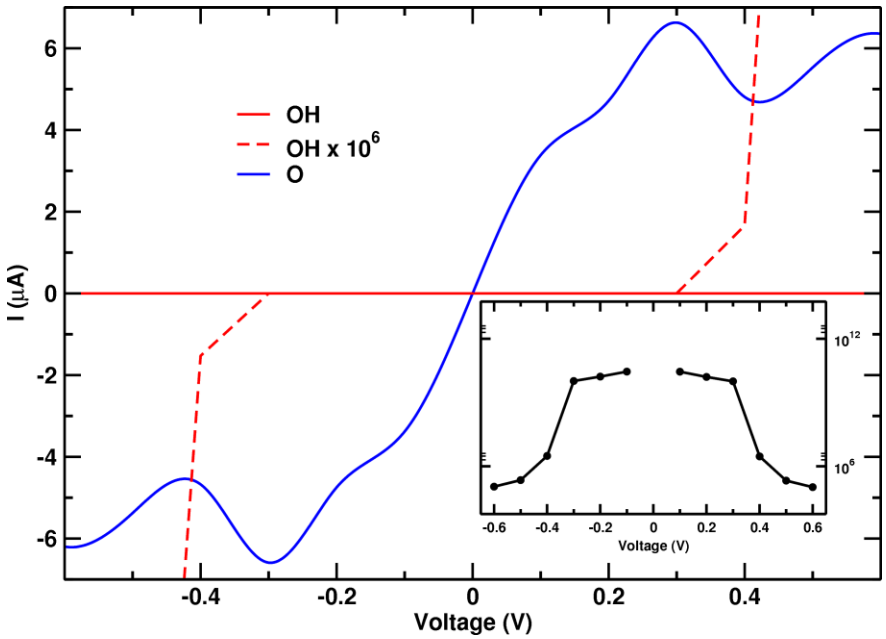

Fig. S7. I(V) characteristics of the switch in Figure 6c-d in the reduced (**7**, continuous red curve) and oxidized (**8**, blue curve) states. A magnification of the values for the reduced state (dashed red curve) by a factor 10^6 is also shown for clarity. Inset: ON/OFF ratio (logarithmic scale).