Supporting Information: Enhancement of Magnetic Stability in Antiferromagnetic CoO Films by Adsorption of Organic Molecules

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1 Temperature dependency of exchange bias with 200 mT cooling field

The temperature evolution for the three samples is shown in figure S1. The three samples were cooled in a magnetic field along the Co easy axis of 200 mT from 300K to 80K.

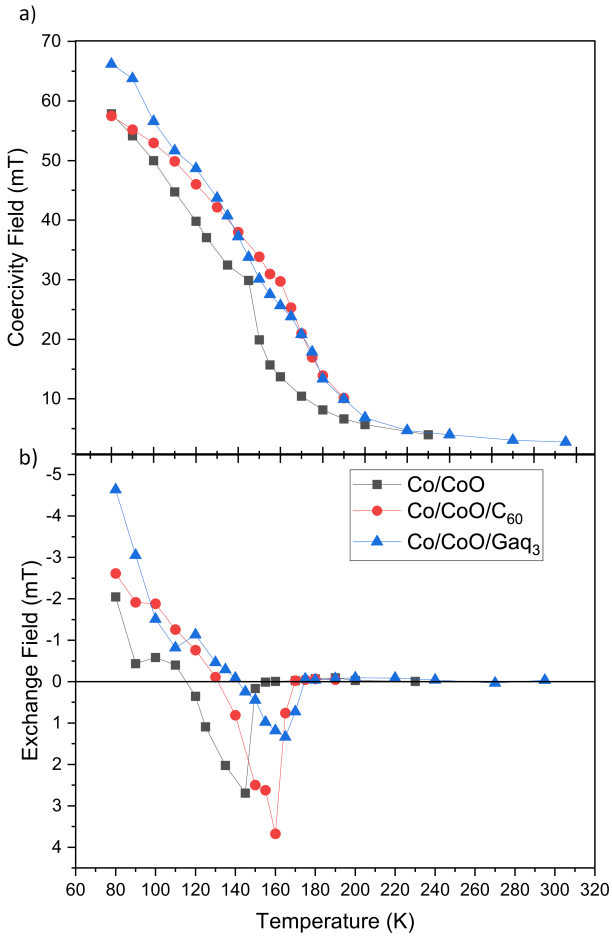

Figure S1: Temperature evolution of coercivity (a) and EB field (b) measured after cooling the three samples in a magnetic field of 200 mT from 300K to 80K

In figure S1, the value of T_P is shifted to higher temperatures with respect to the results obtained with 75 mT cooling field for all the samples.

2 Structural models

The nine configurations of C_{60} on CoO considered as structural model in the theoretical calculations are reported in Figure S2 together with the energy difference with respect to the most stable configuration which is reported in the main text. All the structures have been relaxed.

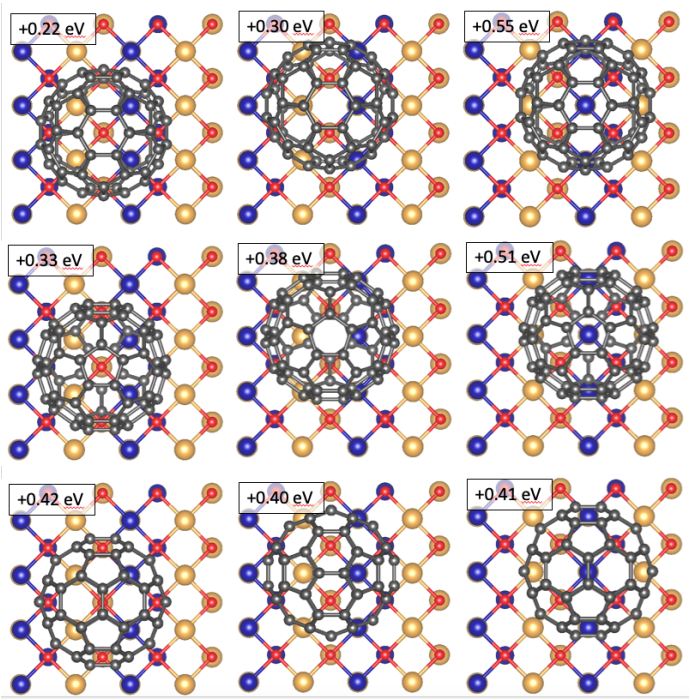

Figure S2: Calculated structural models and energy difference with respect to the most stable configuration reported in the text.

3 Induced charge and magnetic moments

The adsorption of C_{60} molecules on the CoO surface induces a charge redistribution in the surface layer due to the interaction with the molecule. The analysis of the Mulliken charges shows a very small increase of electronic charge (0.099 e/cell) in the surface layer which results from the transfer of electrons to Co atoms (0.14 e/cell) and the depletion of charge on O atoms (-0.083 e/cell). The induced charge on Co atoms is mainly due to a contribution

from the subsurface layer. The adsorption of C_{60} molecules determines a rearrangement of the occupation of the d orbitals, as discussed in the manuscript and a net transfer of electrons from the substrate to the molecule (0.12 e/mol) with the major contribution on the C atoms of the hexagon facingthe surface and a mild charge redistribution on outer C atoms.

The charge transfer is responsible for local variations of the magnetic moments of both O and Co atoms. The major changes are observed at the interface with the molecules while they decay in the bulk (see Fig. S3).

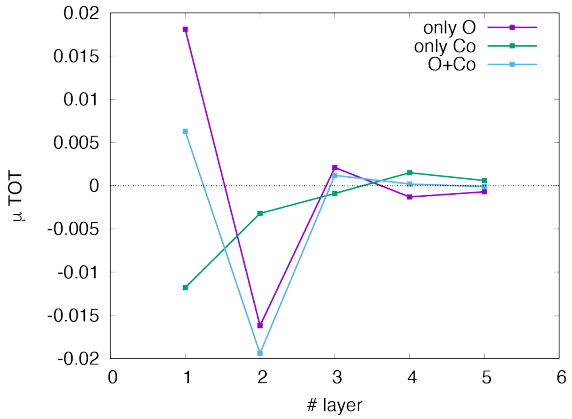

Figure S3: Decay in the substrate of the magnetic moment of O, Co and the sum of the two.

4 PDOS of C_{60} and other species

In Figure S4a is reported the PDOS for the two spin components projected on different atoms, namely on C_{60}, O and Co atoms of the first layer. The spin polarization is very small in the PDOS of C_{60} and O and small differences between the two spin components can not be appreciated. Differently, for Co it is evident the opposite polarization of Co atoms at the surface (blue and green lines). In Figure S4b the total PDOS resolved in m components for the hexagonal face of C_{60} near to the surface in the CoO/C_{60} system is compared with the analogous PDOS for the isolated molecule showing the changes induced by the interaction with the substrate. In Figure S5 is reported the analogous of Figure 7 in the main text but for the majority spin component.

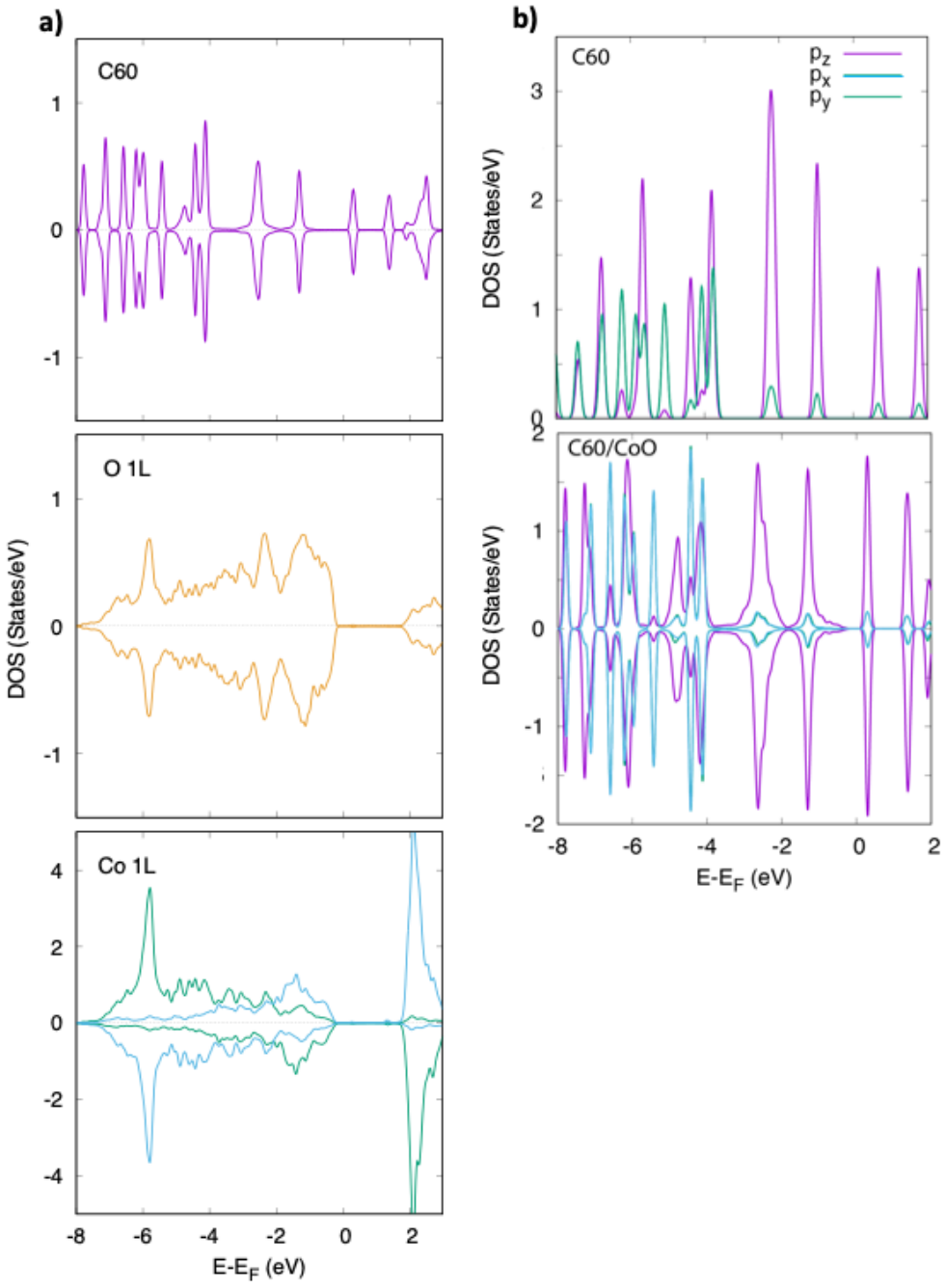

Figure S4: a)PDOS on C_{60} and O and Co atoms of the first layer. For Co, the PDOS of atoms with opposite magnetization are distinguished (blue and green line). b) PDOS of the six carbon atom facing to the surface for CoO/C_{60} and the analogous for C_{60} in gas phase.

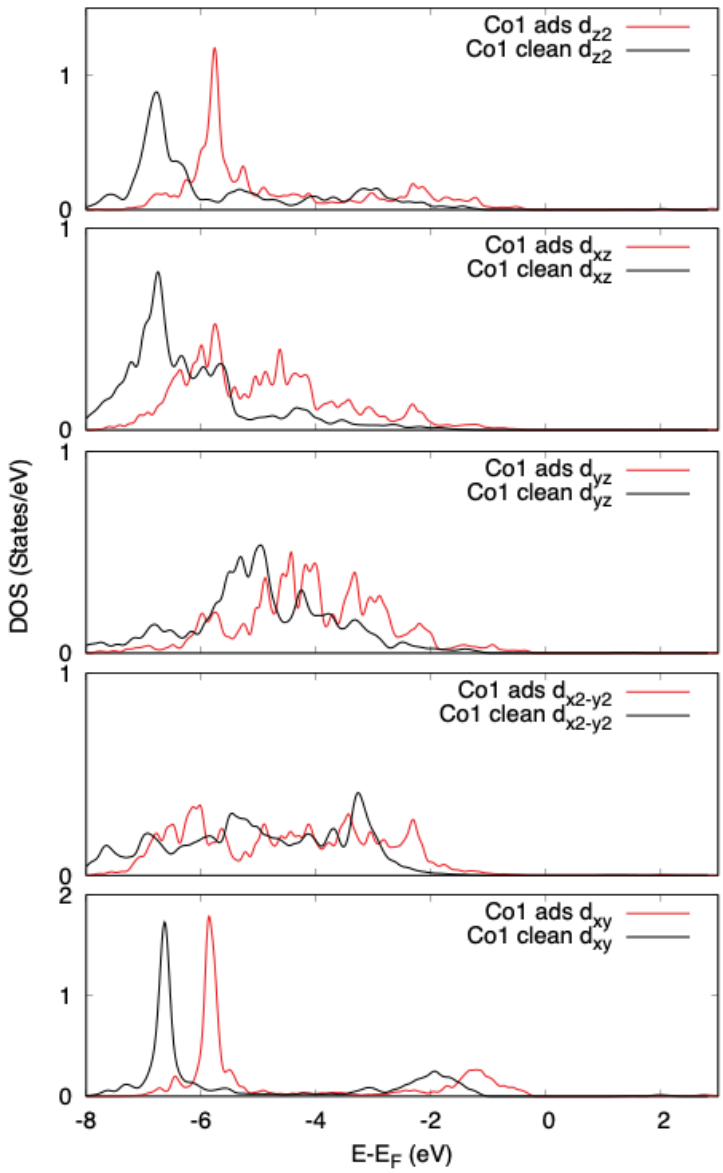

Figure S5: Majority spin density of states of surface Co projected on d orbitals for the C60/CoO (red) and the clean CoO surface (black).