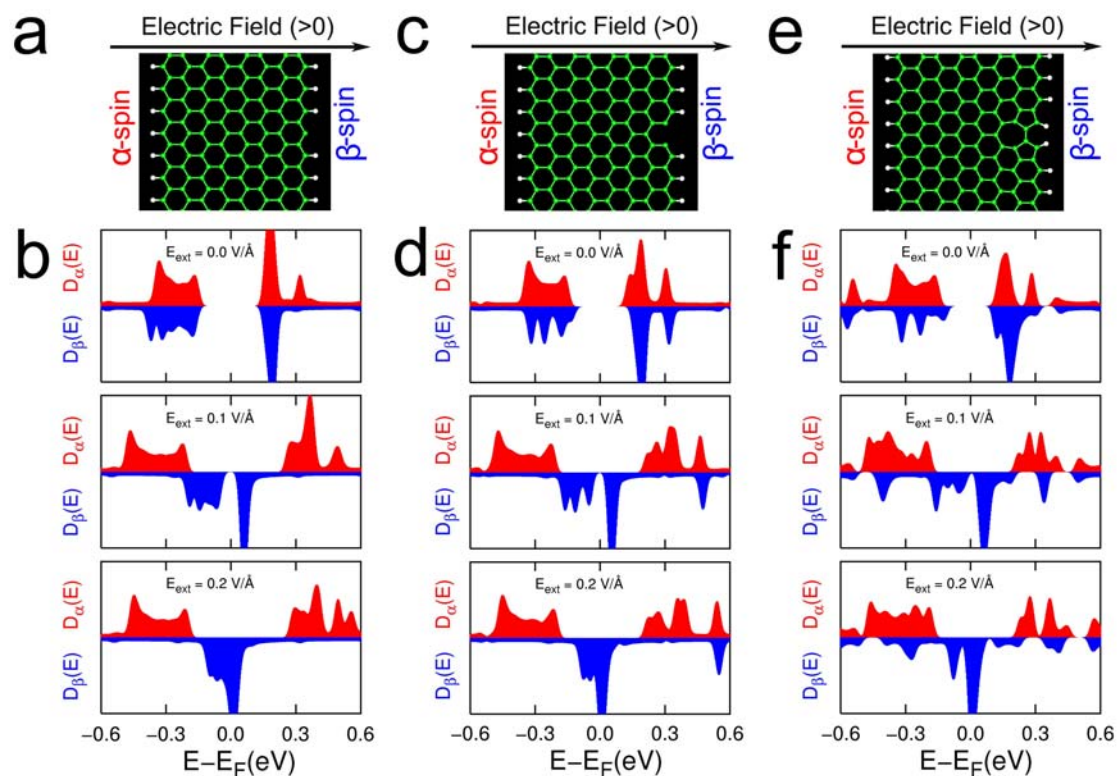


Supplementary Figure and Legend



Supplementary Figure 1. Robustness half-metallicity in defective

graphene nanoribbons. **a**, A ball-and-stick model of an 8-ZGNR with one dangling bond (an edge carbon atom without hydrogen passivation) on the right edge. One dangling bond per 17 edge atoms are considered, which corresponds to 5.9% impurity concentration per one edge. In the figure, the atomic structure near the defect is displayed. Electric fields ($E_{\text{ext}} > 0$) are applied from the left side to the right side. The α -spin state is located on the left side and the β -spin state on the right side in the case of the ground state without applied electric fields. **b**, From top to bottom panels, the spin resolved total density of states (TDOS) are drawn for a defective 8-ZGNR shown in **a** with $E_{\text{ext}} = 0.0, 0.1,$ and 0.2 V/Å respectively. At the same critical E_{ext} of 0.2 V/Å of an

ideal 8-ZGNR, the gap for β -spin state is completely closed. **c**, A ball-and-stick model of an 8-ZGNR with one carbon-atom vacancy on the right edge. Defect concentration, ground spin configuration, and direction of electric fields are identical to the case of an 8-ZGNR with one dangling bond shown in **a**. **d**, The TDOS for an 8-ZGNR with one vacancy on the right edge (shown in **c**) with and without electric fields. Half-metallic nature persists also in this case. **e**. A ball-and-stick model for an 8-ZGNR with one single rotated bond (Stone-Wales defect) at the right edge. Defect concentration per one edge in this case is 11.8% since two edge atoms participate to create a Stone-Wales (SW) defect. Electric fields and ground spin configuration follow the same convention described in **a** and **c**. The total energy of an 8-ZGNR with a SW defect is much higher than that of the ideal one by 3.05 eV per defect so that appropriate treatments (e.g. annealing) on the sample will remove highly unstable defect of this kind. Nevertheless, even with such high defect concentration shown in **e**, the TDOSs displayed in **f** clearly show the robustness of the half-metallicity since the gap for the β -spin states is completely closed while the gap for the α -spin states is at 0.39 eV with $E_{\text{ext}} = 0.2 \text{ V/\AA}$.