Giant unilateral electric field control of magnetic anisotropy in MgO/Rh_2CoSb heterojunctions

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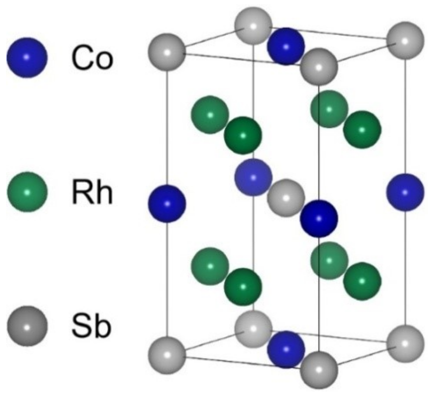

Fig. S1 The crystal structure of Rh_2CoSb. The sites of the lattice with space group *I* 4*/mmm* (139) are occupied as follows: 4*d* (0 1/2 1/4), Rh; 2*b* (0 0 1/2), Co; and 2*a* (0 0 0), Sb.

Table S1 The Rh-O bond lengths and total magnetic moments of MgO/Rh_2...Rh_2 heterojunction under different convergence criterion of ionic relaxations with force less than 10^{-2} eV/ Å .

EDIFF/EDIFFG	10×10^{-6} eV/0.01 eV/Å	10×10^{-7} eV/0.01 eV/Å	10×10^{-8} eV/0.01 eV/Å	10×10^{-8} eV/0.001 eV/Å	10×10^{-8} eV/0.0001 eV/Å
Rh-O bond length	2.28228 Å	2.28294 Å	2.28313 Å	2.28329 Å	2.28273 Å
Total magnetic moment	9.626 μ_B	9.616 μ_B	9.621 μ_B	9.625 μ_B	9.627 μ_B

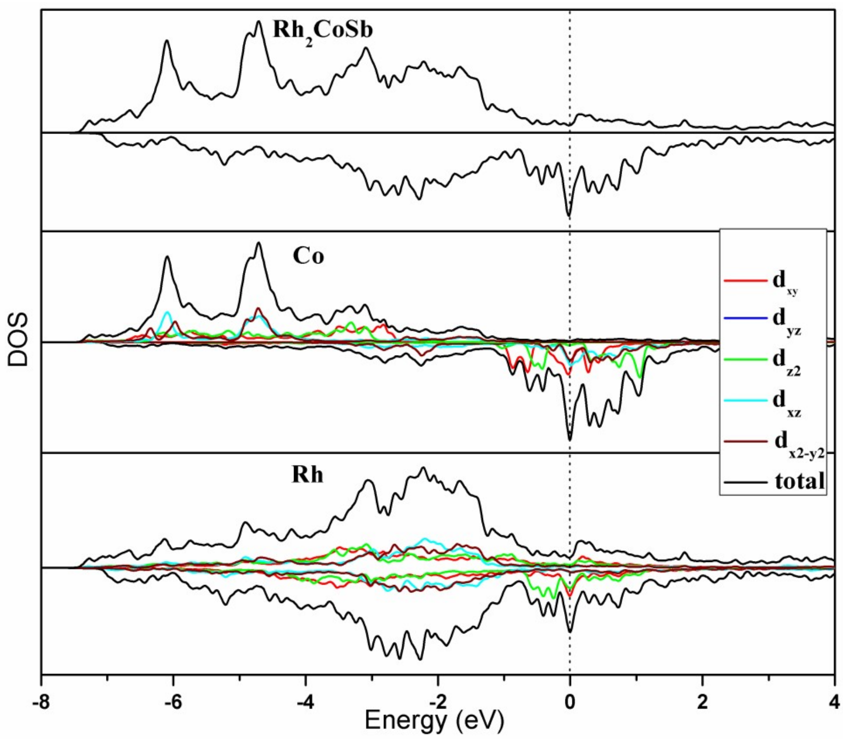

Fig. S2 DOS of Rh_2CoSb (a) and PDOS of Co (b) and Rh (c) in the $MgO/Rh_2...Rh_2$ heterojunction.

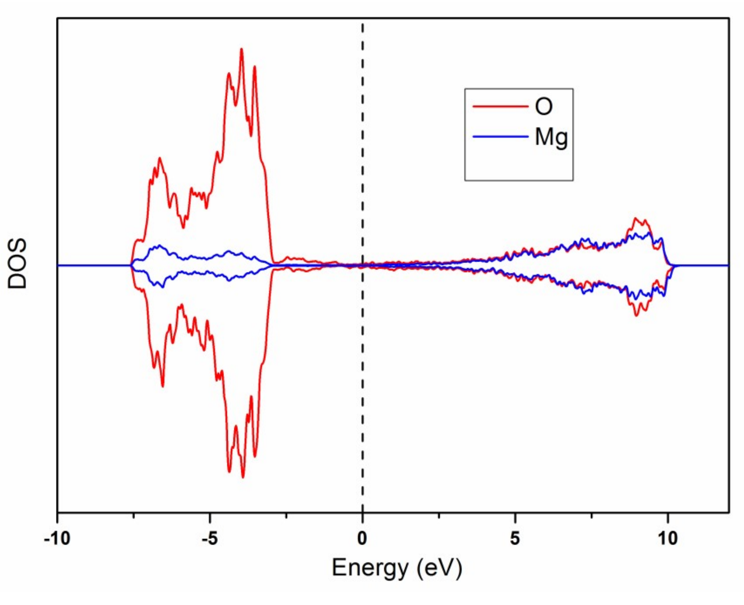

Fig. S3 DOS of MgO in the $MgO/Rh_2...Rh_2$ heterojunction.

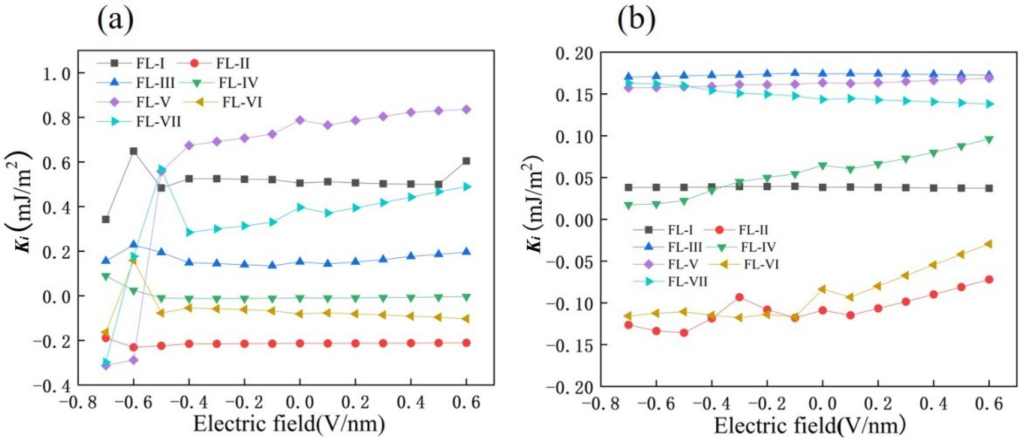

Fig. S4 Layer-resolved K_i of MgO/Rh_2...Rh_2(a) and MgO/Co...CoSb (b) heterojunctions under different electric fields.

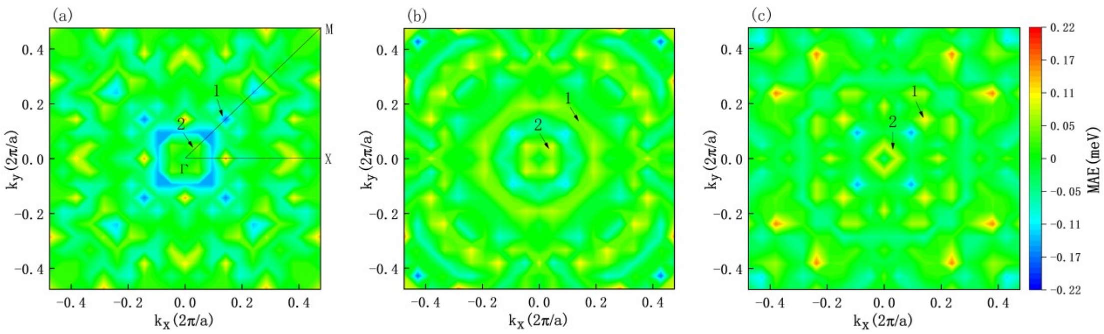

Fig. S5 k-resolved K_i of the fourth-layer Rh atom in the MgO/Co...CoSb heterojunction. (a), (b) and (c) are the electric fields of -0.4 V/Å, 0 V/Å and 0.4V/Å, respectively.

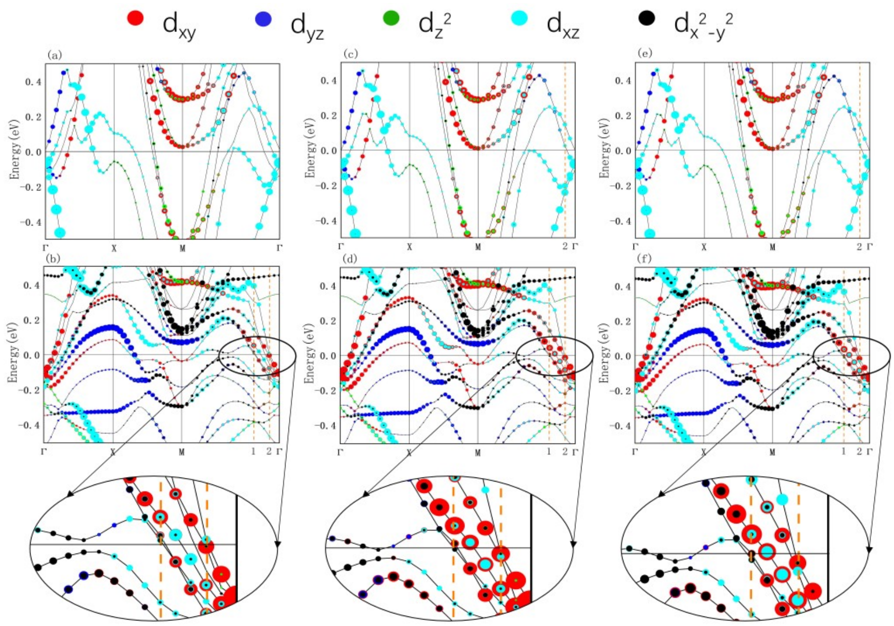

Fig. S6 The d-orbital-projected band structure of the fourth-layer Rh atom in the MgO/Co...CoSb heterojunction. (a), (c) and (e) are in the spin-up state and (b), (d) and (f) are in the spin-down state, under electric fields of -0.4 V/Å, 0 V/Å and 0.4 V/Å, respectively.

In the MgO/Co...CoSb heterojunctions, as shown in Fig. S4 (b), the electric field has a greater effect on Rh atoms in layers 2, 4 and 6, but a weak effect on Co atoms in layers 1, 3, 5 and 7. We chose the fourth-layer with obvious changes to study it. The d-orbital-projected band structures and the k-resolved MAE of the fourth-layer Rh atom in the MgO/Co...CoSb are shown in Fig. S5 and Fig. S6. As shown in Fig. S5(a) and Fig. S6(a), the negative MAE at k point 1 arises from the coupling between the occupied minority-spin state d_{xz} and the unoccupied minority-spin state $d_{x^2-y^2}$ along M-Γ. The negative MAE at k point 2 arises from the coupling between the occupied minority-spin state d_{xy} and the unoccupied minority-spin state d_{xz} along M-Γ. As the electric field increases, the MAE at k points 1 and 2 change from negative to positive, as shown in Fig. S5 (a), (b) and (c). At k point 1, the unoccupied minority-spin state $d_{x^2-y^2}$ orbital near the Fermi level moves downward, and the unoccupied state of $d_{x^2-y^2}$ orbital becomes occupied state, resulting in that negative MAE becomes positive MAE. The positive MAE at k point 1 arises from the coupling between the occupied minority-spin state $d_{x^2-y^2}$ and the unoccupied minority-spin state d_{xy} along M-Γ, as shown in Fig. S6 (d) and (f). At k point 2, the unoccupied minority-spin state d_{xz} orbital near the Fermi surface moves downward, and the d_{xz} orbital becomes the occupied state from the unoccupied state. The positive MAE at k point 2 arises from the coupling between the occupied minority-spin state d_{xy} and the unoccupied majority-spin state d_{xz} along M-Γ, as shown in Fig. S6 (c), (d), (e) and (f).