

Supporting Information

Multiferroicity driven by single-atom adsorption on the two-dimensional semiconductor ScCl_3

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Table S1. The electronic bandgap (G), electric polarization (P) and magnetic anisotropic energy (MAE) of the K@ScCl_3 at different U values.

| K@ScCl_3 | U(eV) | G(eV) | P(pC·m ⁻¹) | MAE(meV) |
|-------------------|-------|-------|------------------------|----------|
| Hollow-1 | 1 | 0.816 | 7.29 | 0.22 |
| | 2 | 0.782 | 7.13 | 0.24 |
| | 3 | 0.752 | 6.91 | 0.26 |
| | 4 | 1.264 | 5.19 | 0.83 |
| | 4.7 | 1.736 | 4.65 | 0.91 |
| | 5 | 1.292 | 4.51 | 0.95 |

Table S2. The adsorption energies of different structures K@ScCl_3 at different U values. The Cl-top structure always automatically converges to the Hollow-1 structure after structural relaxation.

| U(eV) | E_b (eV) | | | | |
|-------------------|------------|----------|--------|--------|--------|
| | Hollow-1 | Hollow-2 | Sc-top | Cl-top | |
| K@ScCl_3 | 1 | -2.022 | -1.884 | -1.272 | -2.022 |
| | 2 | -2.013 | -1.889 | -1.230 | -2.013 |
| | 3 | -1.990 | -1.956 | -1.173 | -1.990 |
| | 4 | -2.083 | -2.056 | -1.138 | -2.083 |
| | 4.7 | -2.184 | -2.203 | -1.106 | -2.184 |
| | 5 | -2.219 | -2.203 | -1.106 | -2.219 |

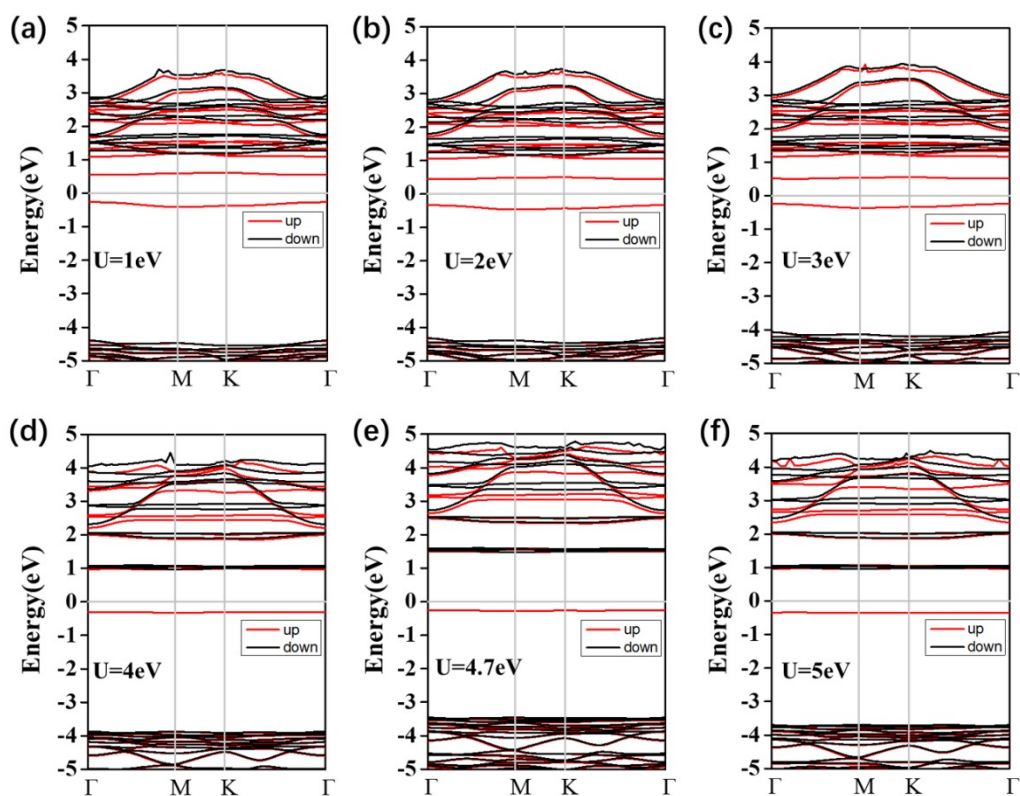


Figure S1. (a-f) The band structures of K@ScCl_3 with U values ranging from 1 to 5 eV.

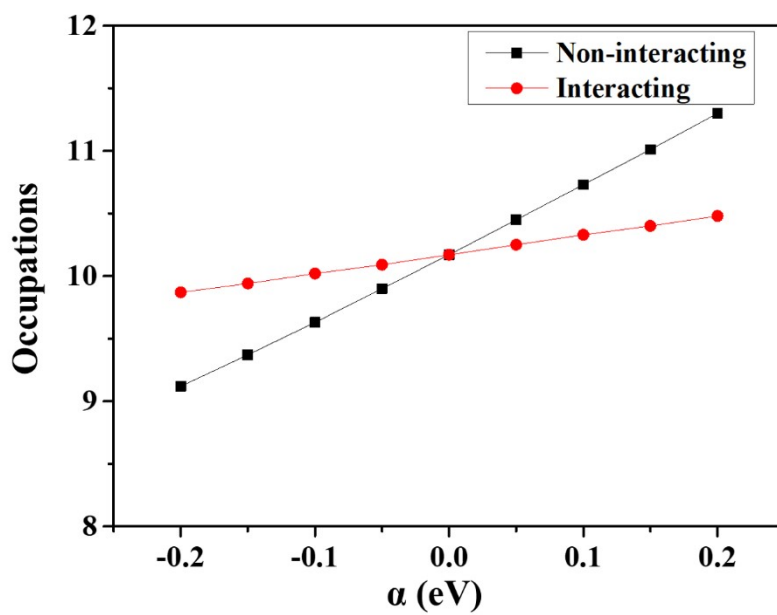


Figure S2. The interacting and non-interacting Kohn-Sham response for K@ScCl_3 .

