Differences in magnetic properties of CrI_3 and $CrBr_3$ monolayers caused by spin-orbit coupling

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After the discovery of magnetism in monolayer CrI_3, the magnetic properties of different two-dimensional materials from the chromium-trihalide family are intuitively assumed to be similar, yielding magnetic anisotropy from the spin-orbit coupling on halide ligands. Here we reveal[1] significant differences between seemingly similar CrI_3 and $CrBr_3$ magnetic monolayers (see Figure 1) in their magnetic anisotropy, resulting Curie temperature, hysteresis in an external magnetic field, and evolution of magnetism with strain, all predominantly attributed to a distinctly different interplay of atomic contributions to spin-orbit coupling in two materials.

REFERENCES

[1] C. Bacaksiz, D. Šabani, R. M. Menezes, and M. V. Milošević, Physical Review B, **103** 125418 (2021).

FIGURES

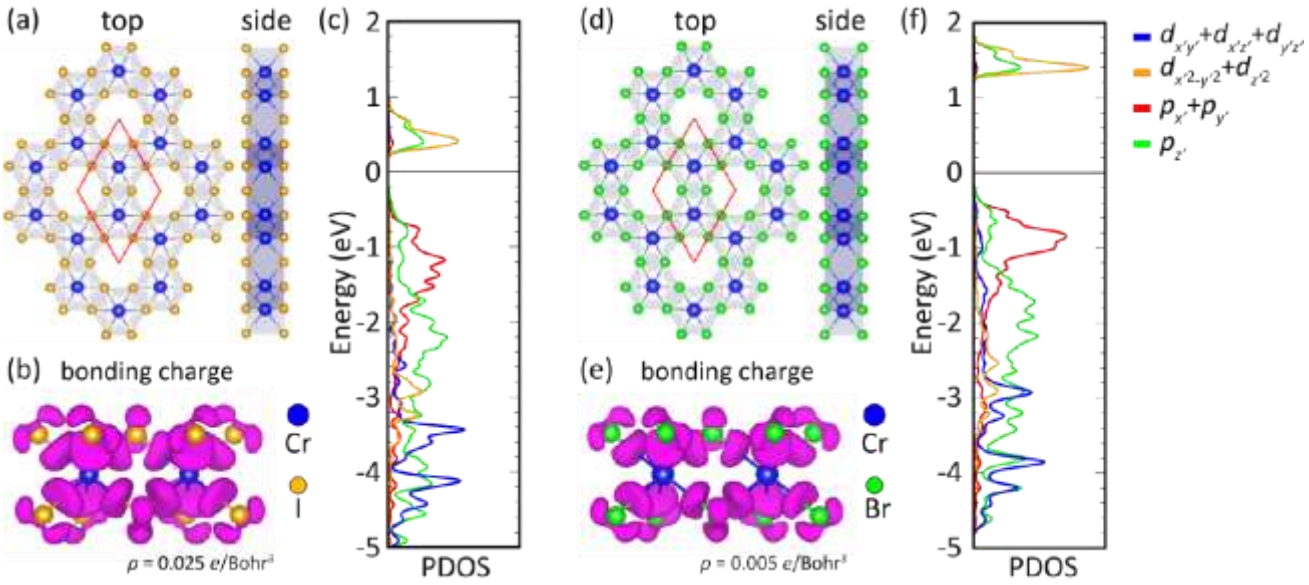

Figure 1: Schematic representation of the structure of monolayer CrI_3 (a) and $CrBr_3$ (d). Panels (b) and (e) show the difference between the charge distribution after crystallization and the total charge distribution of bare atoms, which then indicates the bonding and antibonding charges in the two materials. Panels (c) and (f) show the density of states of two materials, decomposed according to the atomic orbitals. Subscripts x′, y′, and z′ in the orbitals denote the local coordinates of the corresponding atoms.