Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material for Strain-tunable magnetic and electronic properties of $CuCl_3$ monolayer

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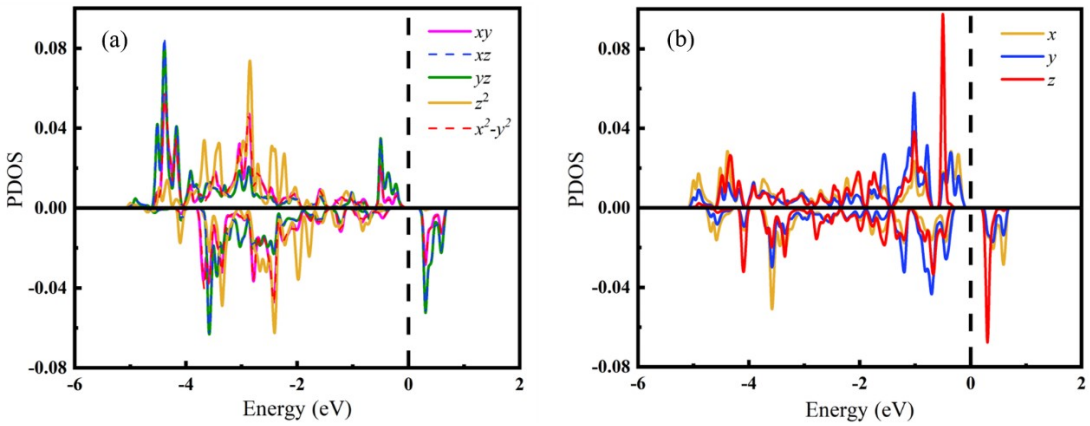

Fig. S1. (a) The *d* orbital PDOS of Cu atom and (b) the *p* orbital PDOS of Cl atom.

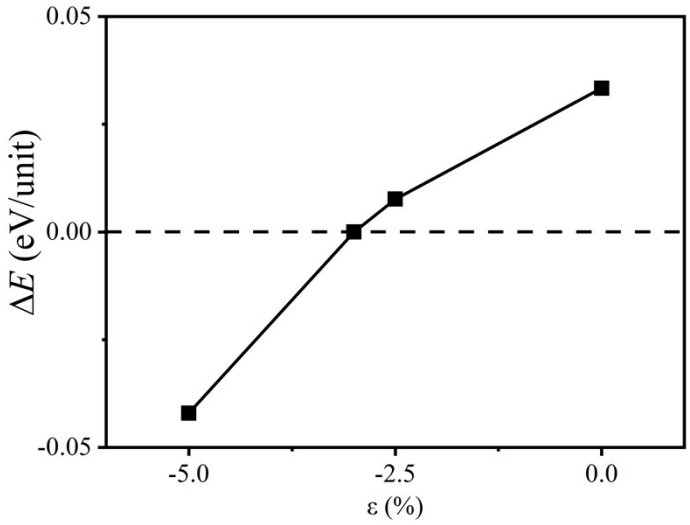

Fig. S2. Energy difference between FM and AFM $CuCl_3$ monolayer as a function of the strain calculated by the LSDA.

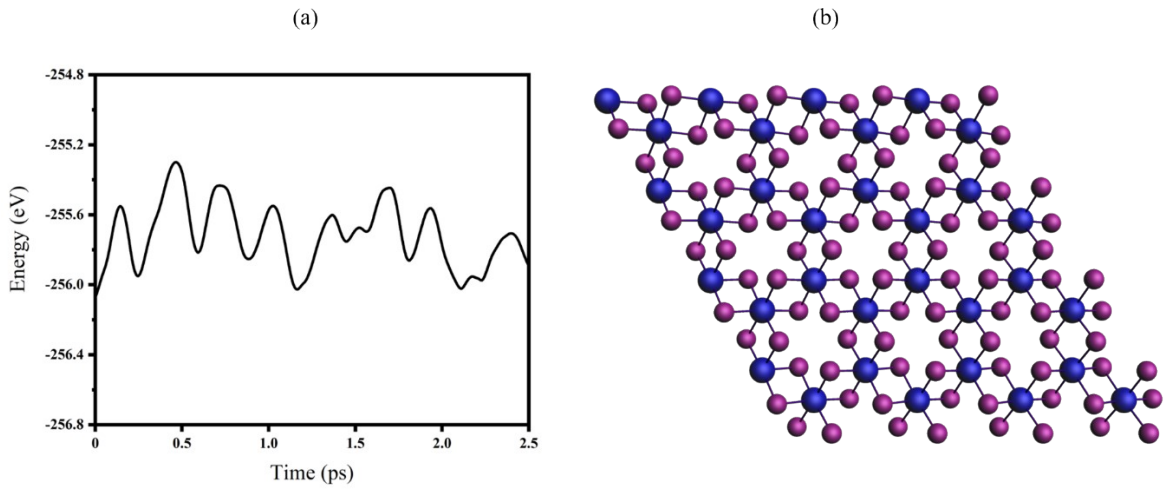

Fig. S3. (a) The potential energy fluctuation during the AIMD simulation at 300 K and (b) the top view of the atomic configuration of 4×4×1 $CuCl_3$ monolayer after 2.5 ps.