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.