Supplementary data

Exploitation of Mixed-Valency Chemistry for Designing Monolayer with Double Ferroelectricity and Triferroic Couplings

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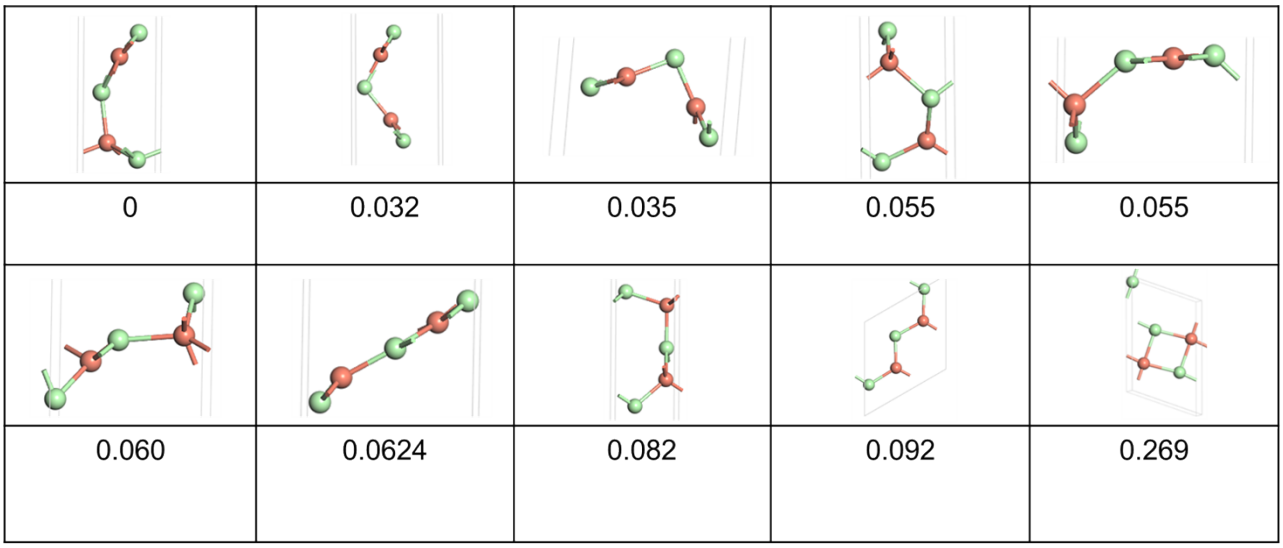

Figure S1. A series of low-energy 2D Cu_2Cl_3 structures obtained in the extensive structural search using the Calypso code, and their relative energies (in eV/f.u. compared with the ground state).

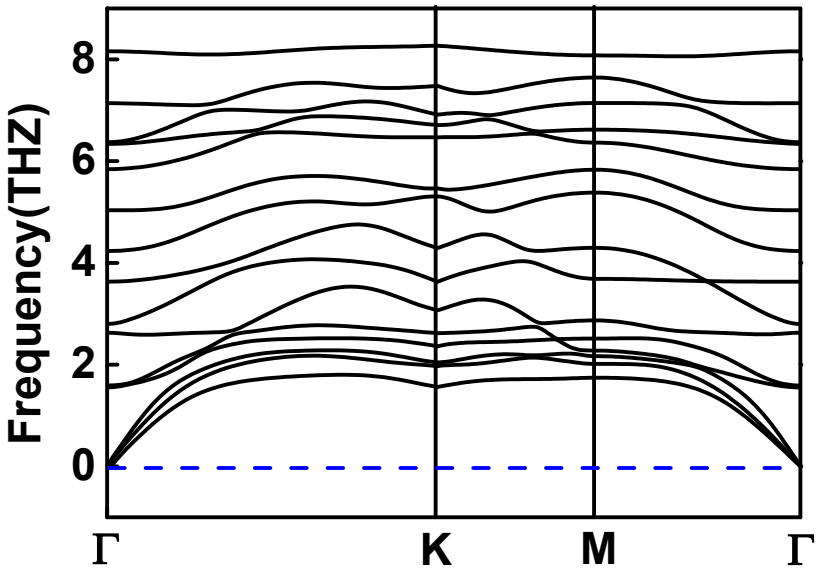

Figure S2. Phonon dispersion of Cu_2Cl_3 monolayer.

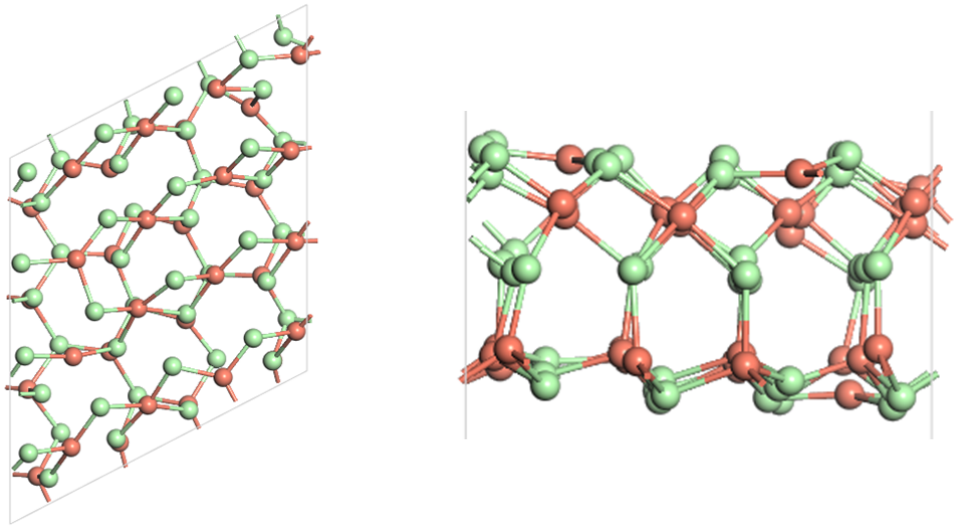

Figure S3. Snapshot of Cu_2Cl_3 monolayer after AIMD simulation in the canonical ensemble at 373K for 15 ps.

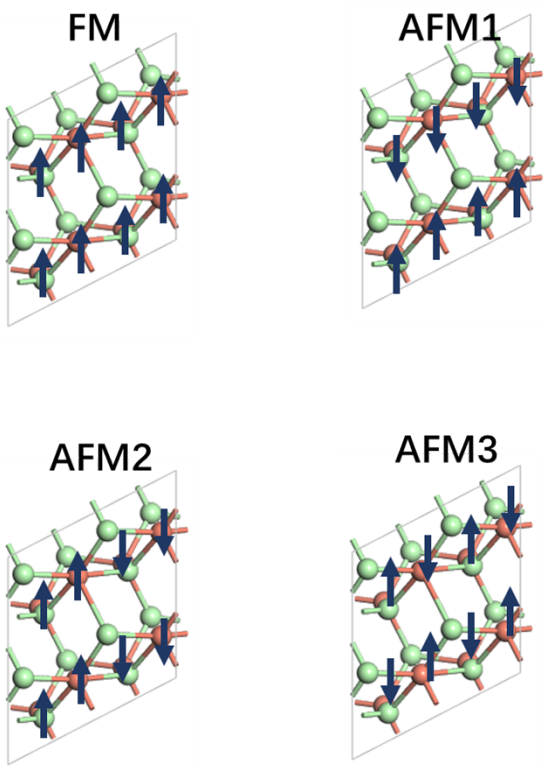

Figure S4. Different spin configurations for Cu_2Cl_3 monolayer, where AFM1, AFM2, AFM3 are respectively 38, 36 and 38 meV higher in energy compared with the FM ground state.