

Supplementary Information

Strain-Tunable Antiferroelectricity in 2D CuCrP₂S₆ for High-Performance Neuromorphic Devices

Dimuthu Wijethunge^{a,b}, Aijun Du^{c,d}*

^a School of Engineering, University of Southern Queensland, 37 Sinnathamby Blvd,
Springfield Central, QLD 4300, Australia.

^b Centre for Future Materials, University of Southern Queensland, Springfield, QLD, 4300
Australia.

*E-mail: Dimuthu.HerathMudiyanselage@unisq.edu.au

^c School of Chemistry and Physics, Queensland University of Technology (QUT), Gardens
Point Campus, 2 George Street, Brisbane, QLD, 4001 Australia.

^d QUT Centre for Materials Science, Queensland University of Technology (QUT), Gardens
Point Campus, 2 George Street, Brisbane, QLD, 4001 Australia

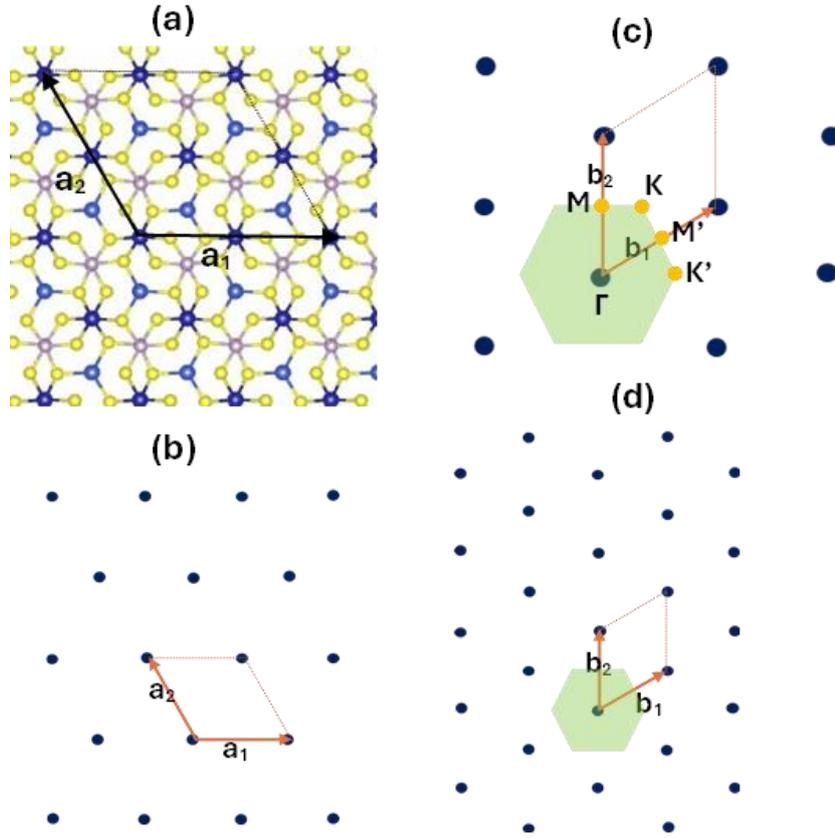


Figure S1: (a) and (b) Real-space representation of the hexagonal lattice. (c) The first Brillouin zone of the hexagonal lattice is shown in green, with high-symmetry points (orange dots). (d) The transformed lattice in reciprocal space is shown, with the corresponding first Brillouin zone highlighted in green.

Table S1: Total energies of the AFE-II and AFE-I configurations under both compressive and tensile strain applied along the a and b-directions.

Strain	AFE-I (a-direction)	AFE-I (b-direction)	AFE-II
-0.04	-201.512	-201.493	-201.352
-0.03	-201.754	-201.741	-201.59
-0.02	-201.923	-201.915	-201.755
-0.01	-202.021	-202.017	-201.853
0	-202.052	-202.052	-202.052
0.01	-202.02	-202.025	-201.857
0.02	-201.929	-201.939	-201.771
0.03	-201.781	-201.799	-201.631
0.04	-201.581	-201.609	-201.44