Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information for: A Copper-Based 2D Hybrid Perovskite Solar Absorber as a Potential Eco-Friendly Alternative to Lead Halide Perovskites

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Contents:

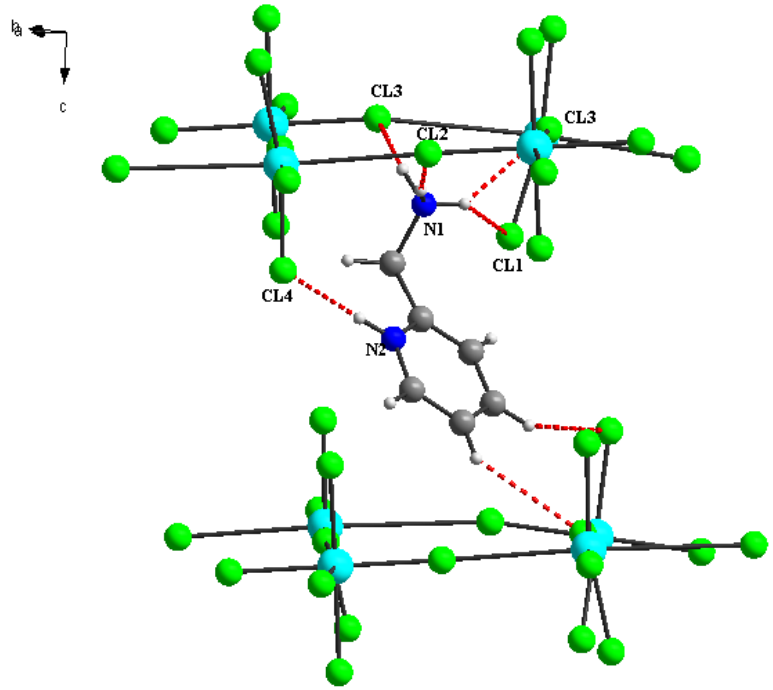

Figure S1. Fragment of the crystal structure, showing the C/N-H...Cl hydrogen bonds for one orientation of the disordered 2-(aminomethyl) pyridindium cation.

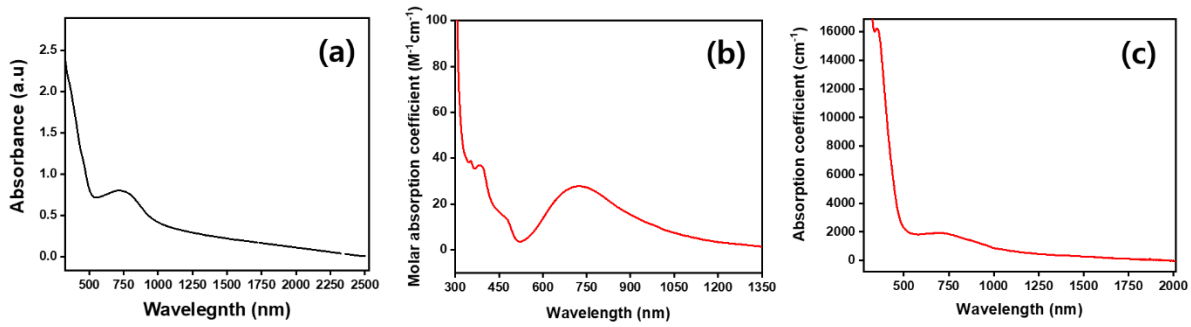

Figure S2. UV-vis absorption spectra of AMP[$CuCl_4$] (a) film (b) molar absorption coefficient vs wavelength, (c) absorption coefficient vs wavelength.

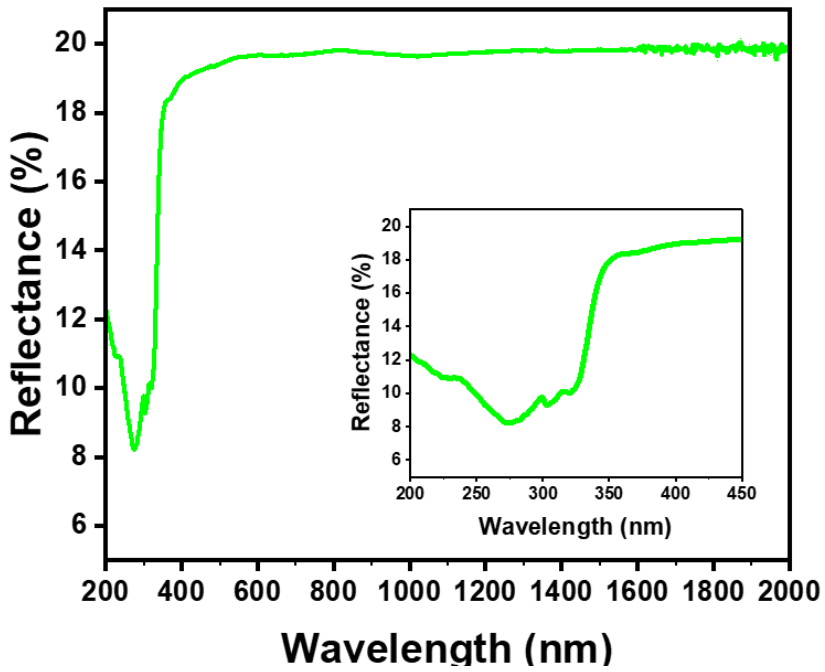

Figure S3. Specular reflectance of AMP[$CuCl_4$].

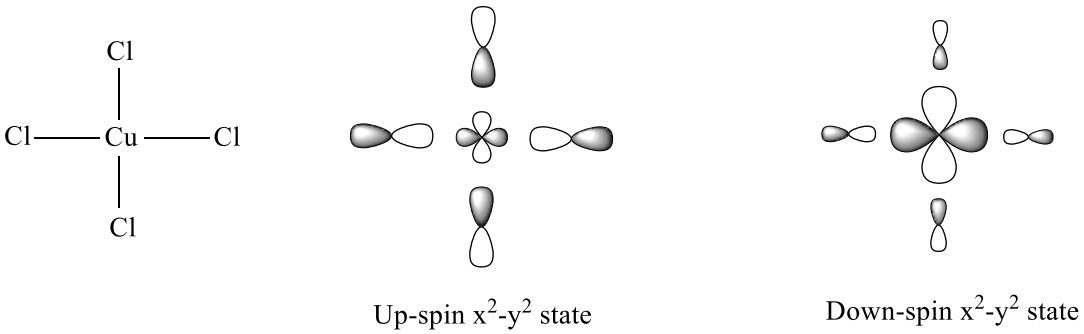

Figure S4. Out-of-phase combinations of the Cu x^2-y^2 and Cl p orbitals in the up-spin and down-spin states of a square planar $CuCl_4$ unit.

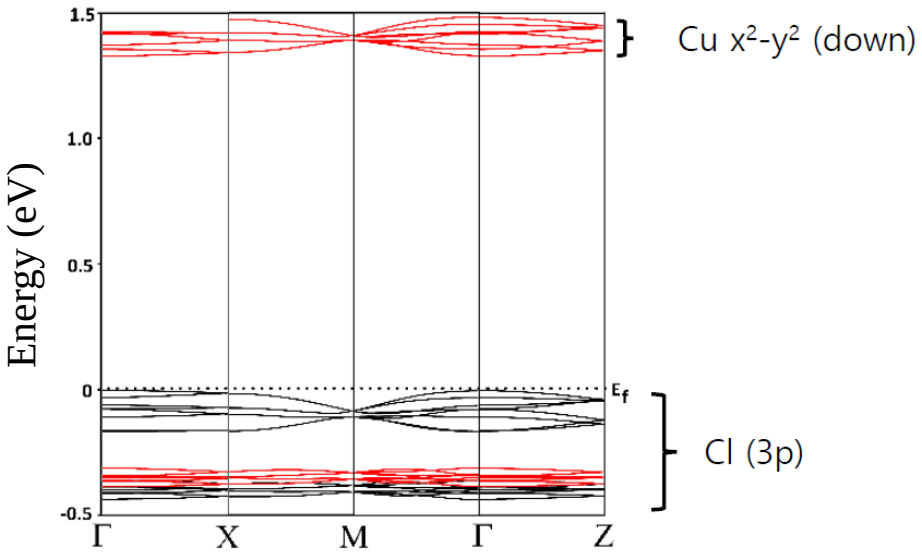

Figure S5. Band dispersion diagram. Red lines correspond to down spins, while black lines correspond to up spins.

Table S1. Selected bond distances (Å) and angles (°) for AMP[$CuCl_4$]

Within the inorganic moiety		**Within the organic moiety**	
Cu - Cl1	2.2705 (12)	N2-C6	1.338(5)
Cu - Cl2	2.2871 (12)	C1-N1	1.480(5)
Cu - Cl3	2.2872 (11)	C1-C2	1.505(6)
Cu - Cl4	2.2881 (12)	C2-N2	1.338(5)
Cl1 – Cu - Cl3	90.09 (4)	C2-C3	1.368(6)
Cl2 – Cu - Cl1	90.72(4)	C3-C4	1.383(6)
Cl2 – Cu - Cl3	177.13(4)	C5-C6	1.362(6)
Cl2 – Cu - Cl4	90.74(4)	C4-C5	1.381(6)
Cl4 – Cu - Cl1	168.86(4)	C6-N2	1.338(5)
		N1-C1-C2	112.5(3)
		N2-C2-C3	118.7(4)
		N2-C2-C1	116.8(4)
		N2-C6-C5	119.9(4)
		C3-C2-C1	124.5(4)
		C2-C3-C4	120.2(4)
		C5-C4-C3	119.1(4)
		C6-C5-C4	119.3(4)

Table S2. Hydrogen-bond geometry (Å,°)

D*—H···*A	***D*—H**	**H···*A***	***D*···*A***	***D*—H···*A***
N1—H1*A*···Cl3^{i}	0.99 (5)	2.26 (5)	3.152 (4)	150 (4)
N1—H1*B*···Cl2^{ii}	0.84 (4)	2.40 (5)	3.225 (4)	171 (4)
N1—H1*C*···Cl1^{iii}	0.91 (4)	2.78 (4)	3.400 (4)	127 (3)
N1—H1*C*···Cl3^{iii}	0.91 (4)	2.43 (4)	3.174 (4)	140 (4)
C1—H2*A*···Cl2	0.99	2.92	3.611 (4)	127
C1—H2*B*···Cl1^{iii}	0.99	2.95	3.544 (4)	119
C3—H4···Cl1^{iii}	0.95	2.88	3.703 (4)	145
C5—H6···Cl2^{iv}	0.95	2.91	3.738 (5)	146
C5—H6···Cl3^{v}	0.95	2.83	3.505 (4)	129
C6—H7···Cl1^{iv}	0.95	2.63	3.564 (4)	167
N2—H8···Cl4	0.90 (4)	2.17 (4)	3.060 (4)	171 (4)
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Symmetry codes: (i) $-x+1, y-1/2, -z+3/2$; (ii) $-x+1, y+1/2, -z+3/2$; (iii) $x+1/2, y, -z+3/2$; (iv) $x, -y+3/2, z-1/2$; (v) $-x+1, -y+2, -z+1$.

Table S3. Hall effect measurement

	Sample 1	Sample 2	Sample 3	Sample 4	Sample 5	Average
Mobility (cm^2/Vs)	12.44	15.63	13.10	18.45	14.41	14.81
Bulk concentration (cm^{-3}) $x10^{14}$	1.72	1.21	1.78	1.33	1.54	1.52
Resistivity (ohm cm) $x10^3$	2.92	3.29	2.6	2.54	2.81	2.85
Applied current (uA)	0.1	0.1	0.1	0.1	0.1	0.1
Magnetic field (Tesla)	0.55	0.55	0.55	0.55	0.55	0.55