Disclosing the Structural, Electronic, Magnetic, and Morphological Properties of $CuMnO_2$: A Unified Experimental and Theoretical Approach

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Supporting Information

Table S1. The heat treatment temperatures and times utilized to obtain $CuMnO_2$ powders.

Code	Temperature (°C)	Time (min)
CM100-1	100	1
CM120-1	120	1
CM140-1	140	1
CM100-5	100	5
CM120-5	120	5
CM140-5	140	5
CM100-10	100	10
CM120-10	120	10
CM140-10	140	10

Table S2. The structural parameters obtained by the Rietveld refinement for the $CuMnO_2$ samples.

Sample	*a* (Å)	*b* (Å)	*c* (Å)	Beta (Degrees)	Volume ($Å^3$)	Crystallite size (nm)	Microstrain (10^{-3})	χ^2	Rp (%)	Rf^2 (%)
CM100-1	5.551	2.886	5.895	104.4	91.5	7.6	3.95	1.258	9.49	16.76
CM120-1	5.570	2.885	5.894	104.2	91.8	14.2	1.78	1.187	9.40	17.34
CM140-1	5.575	2.885	5.893	104.1	91.9	13.7	1.84	1.168	9.49	14.42
CM100-5	5.555	2.886	5.894	104.3	91.6	11.1	2.39	1.162	9.55	16.46
CM120-5	5.572	2.886	5.895	104.2	91.9	12.6	2.09	1.152	9.12	15.50
CM140-5	5.571	2.889	5.901	104.3	92.1	12.4	1.99	1.085	10.2	18.32
CM100-10	5.563	2.887	5.898	104.3	91.8	11.0	2.80	1.199	9.80	18.72
CM120-10	5.570	2.886	5.896	104.2	91.9	13.1	2.02	1.148	9.27	14.96
CM140-10	5.575	2.885	5.895	104.1	91.9	15.4	1.66	1.103	9.09	13.84

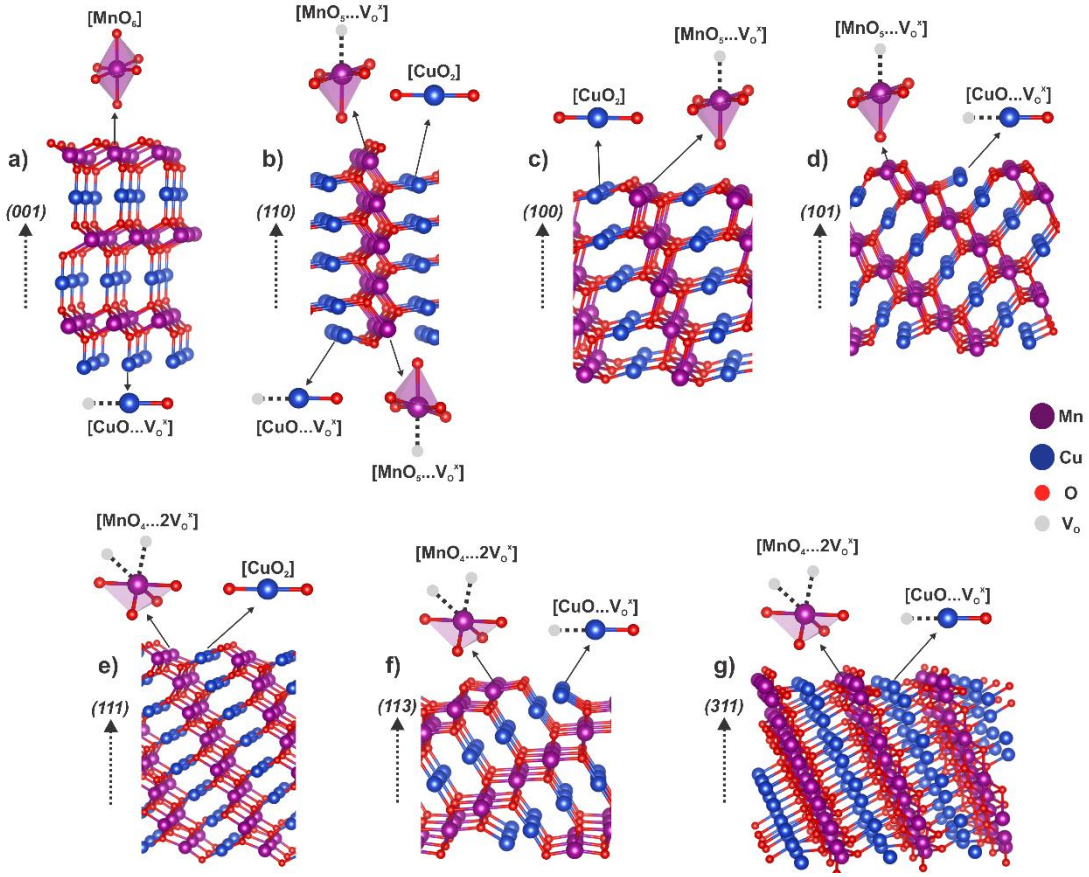

Figure S1. Schematic 3D representations for (001), (100), (101), (110), (111), (113) and (311) surfaces of the $CuMnO_2$. The Cu and Mn local coordination along the exposed surfaces are depicted.

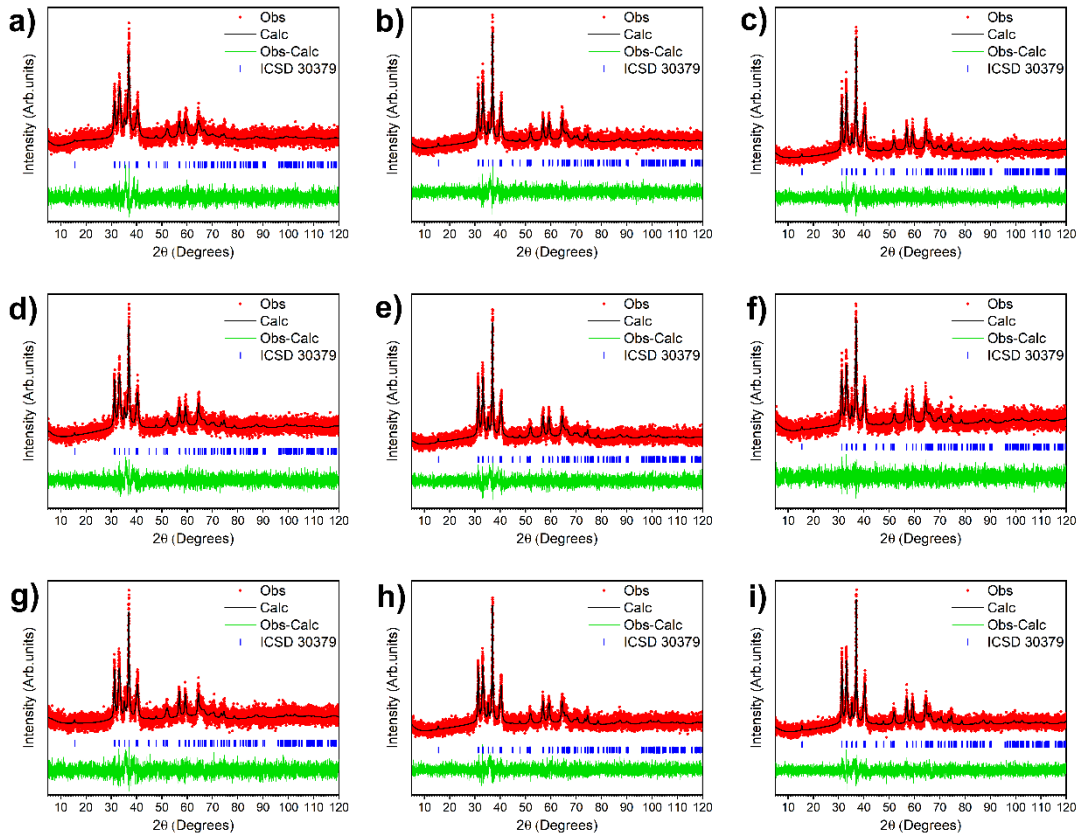

Figure S2. Rietveld refinement graphs for the $CuMnO_2$ samples being (a) CM100-1, (b) CM120-1, (c) CM140-1, (d) CM100-5, (e) CM120-5, (f) CM140-5, (g) CM100-10, (h) CM120-10, and (i) CM140-10.

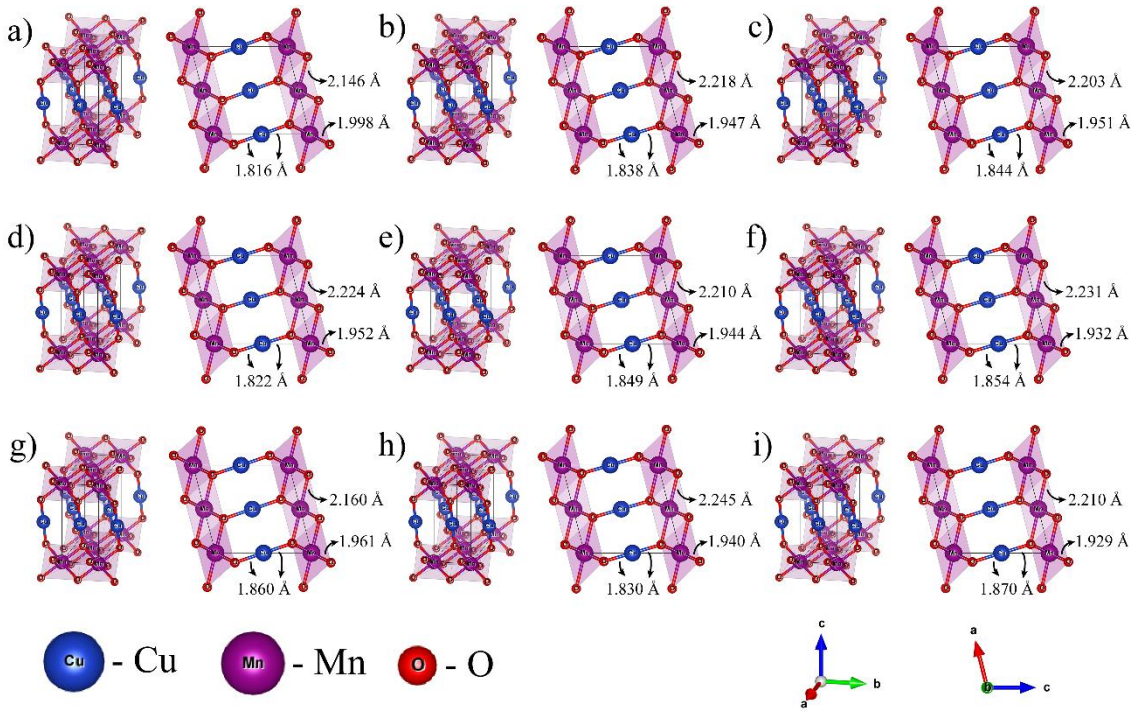

Figure S3. Monoclinic unit-cell of $CuMnO_2$ samples, namely: (a) CM100-1, (b) CM120-1, (c) CM140-1, (d) CM100-5, (e) CM120-5, (f) CM140-5, (g) CM100-10, (h) CM120-10, and (i) CM140-10.

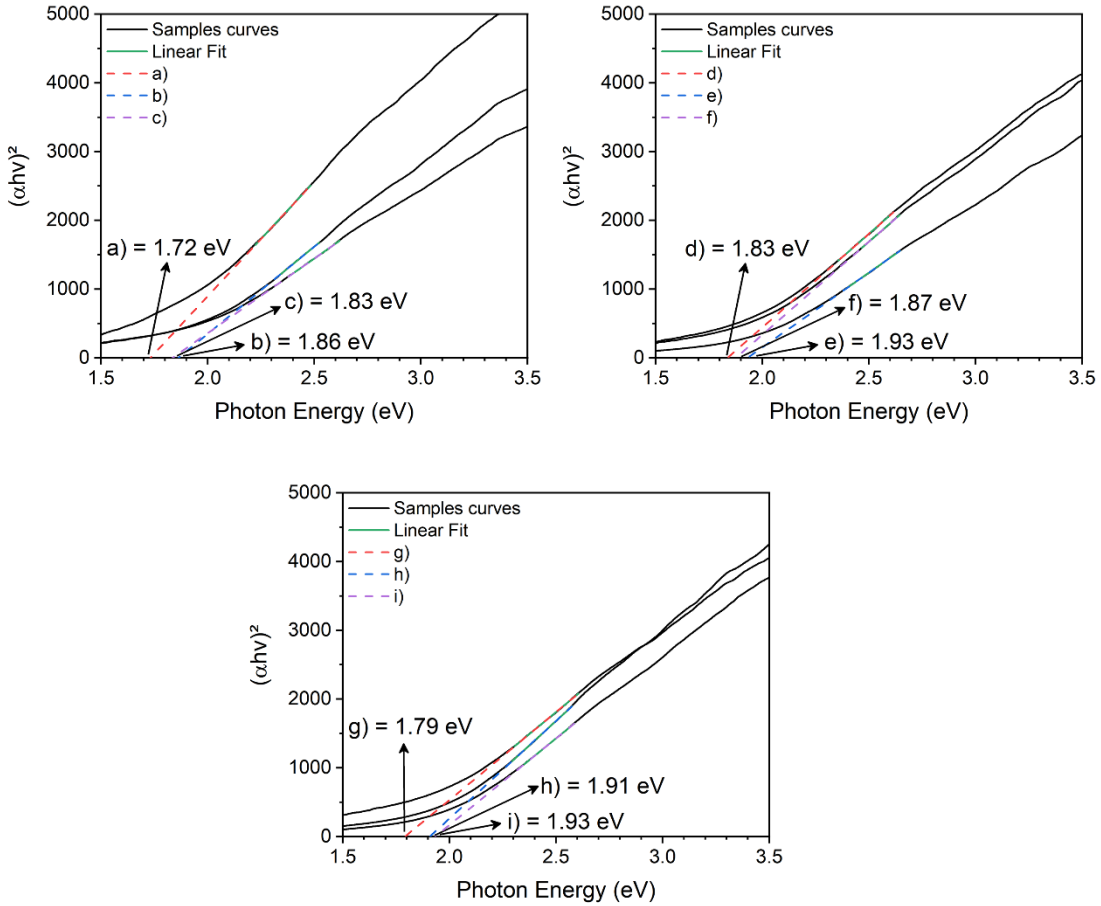

Figure S4. Bandgap values for the $CuMnO_2$ samples, namely: (a) CM100-1, (b) CM120-1, (c) CM140-1, (d) CM100-5, (e) CM120-5, (f) CM140-5, (g) CM100-10, (h) CM120-10, and (i) CM140-10.

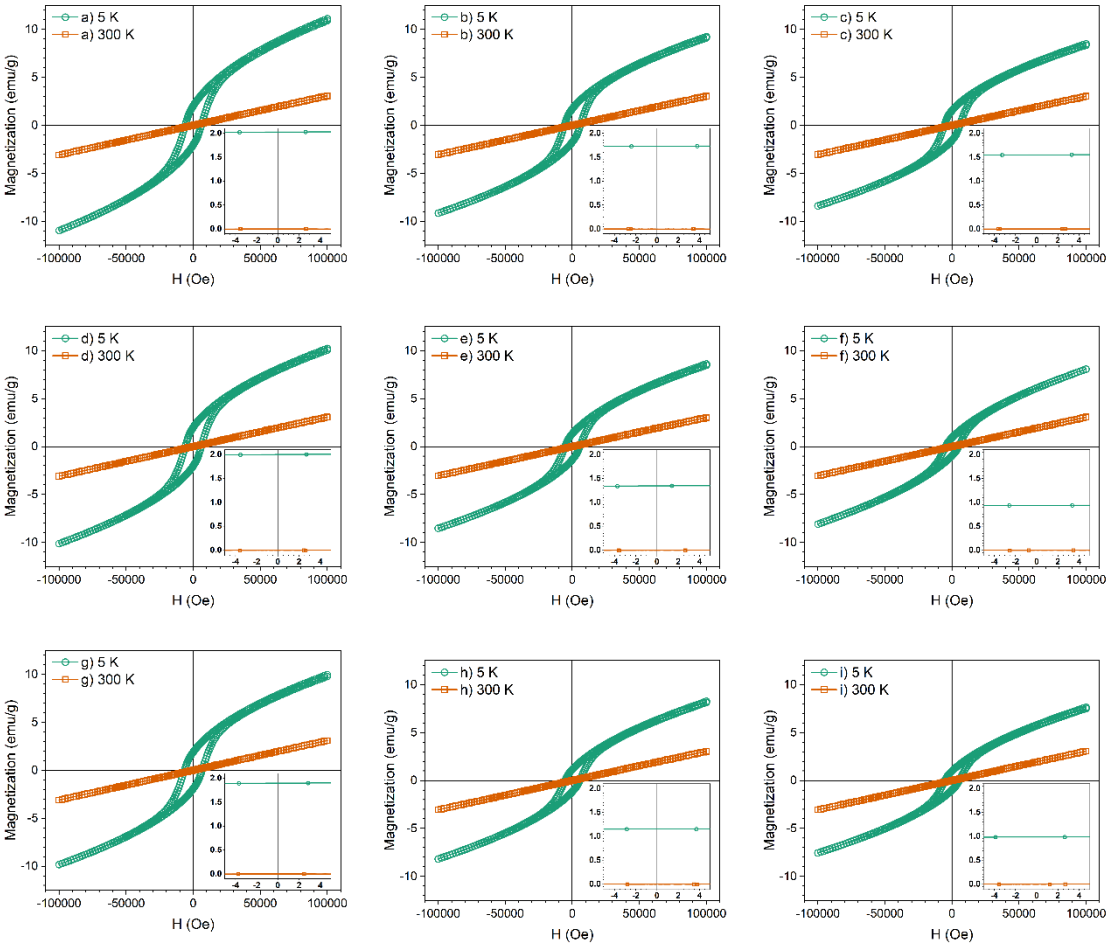

Figure S5. Magnetization curves measured at 5 K and 300 K for the $CuMnO_2$ samples, namely: (a) CM100-1, (b) CM120-1, (c) CM140-1, (d) CM100-5, (e) CM120-5, (f) CM140-5, (g) CM100-10, (h) CM120-10, and (i) CM140-10.

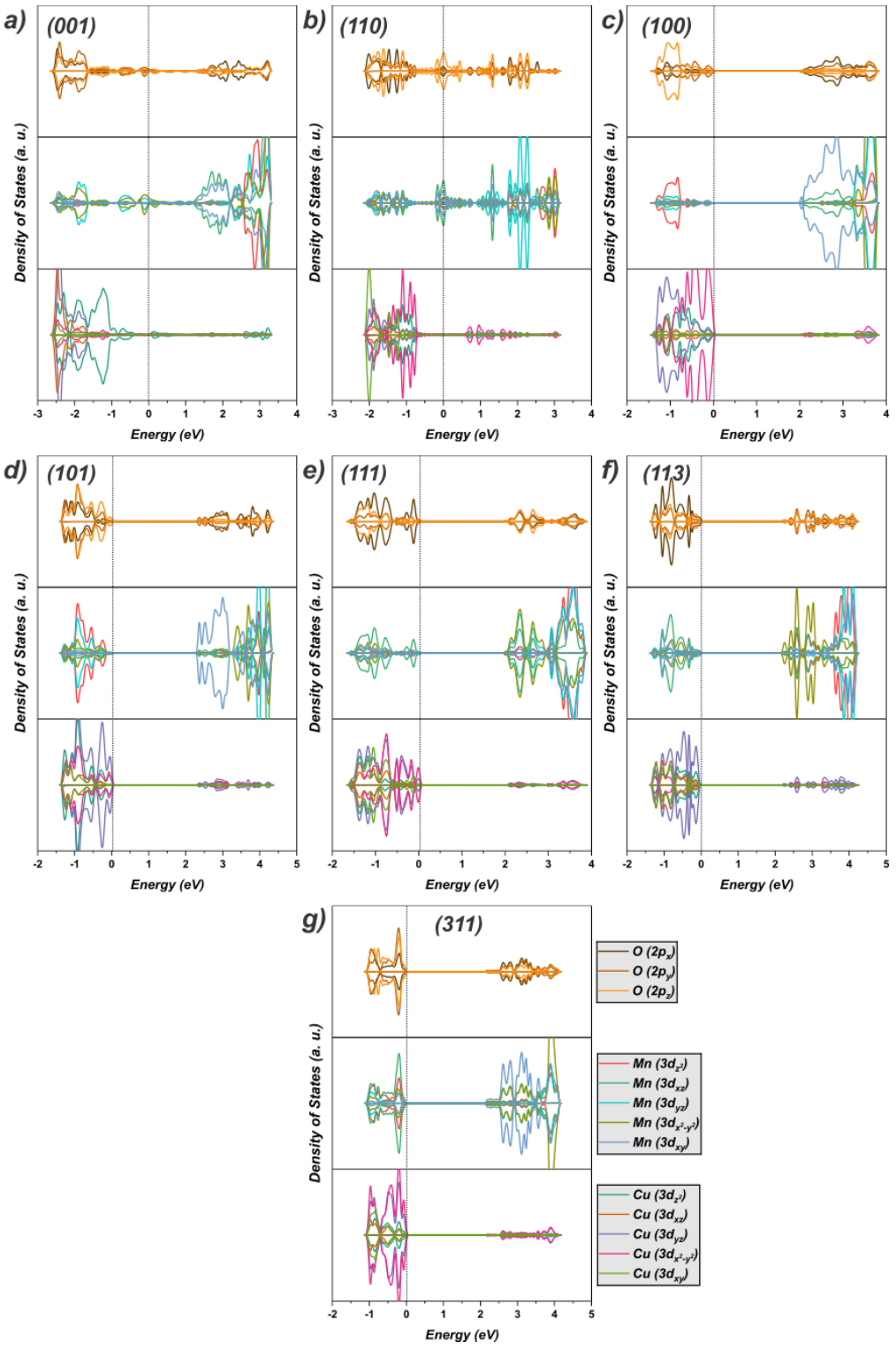

Figure S6. Results of the orbital-resolved DOS profiles for the a) (001), b) (110), c) (100), d) (101), e) (111), f) (113), g) (311) $CuMnO_2$ surfaces.