Supporting information

Screened coulomb hybrid DFT investigation on band gap and optical absorption predictions of CuVO₃, CuNbO₃ and Cu₅Ta₁₁O₃₀ materials

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SEM observations and specific surface area

Field-emission scanning electron microscopy (FE-SEM) was used to investigate the size and morphology of the products. SEM images (Figure S1) were taken on a Quanta 600 electron microscope operated at 5 kV.



Figure S1. SEM images of (a) Cu₂O, (b) CuVO₃, (c) CuNbO₃, (d) Cu₅Ta₁₁O₃₀.

SEM images of Cu₂O precursors (Figure S1a) indicated a large particle size of ~5 μ m. The single CuVO₃ phase contained multifaceted spherical particles with an average size of ~2 μ m, as shown in Figure S1b. The nitrogen adsorption-desorption isotherm of CuVO₃ recorded was Type I according to the IUPAC classification, indicating the non-porous nature of the materials. The specific surface area was calculated by the Brunauer–Emmett–Teller (BET) equation. Given the non-porous nature of the product, the specific

Upon complete crystallization to the CuNbO₃ phase, vesicle-like morphologies were evident, as shown in the SEM image shown in Figure S1c. The dimensions of the particles

surface area was approximately $5 \text{ m}^2 \text{ g}^{-1}$.

increased with fusions that occurred with increasing solid-state reaction temperature, and the average size of the final CuNbO₃ particles was approximately $2 \times 10 \ \mu\text{m}$. CuNbO₃ also exhibited Type I nitrogen adsorption-desorption isotherms, indicating the non-porous nature of the material. The specific surface area calculated by the BET equation was low (3-4 m² g⁻¹) in the case of the CuNbO₃ samples.

Cu(I) tantalate particles were fused into large lumps when the solid-state synthesis temperature was increased further, as shown in Figure S1d. In accordance with the trend in the sharpness of the XRD patterns, large particles of up to 50 μ m were observed for the highly crystalline Cu(I) tantalate. The nitrogen sorption isotherms of Cu(I) tantalate also indicated that the material was non-porous. The solid-state reaction temperature for the synthesis of Cu(I) tantalate was the highest among the group-V transition metals. The BET specific surface area of the Cu(I) tantalate (approximately 2 m² g⁻¹) was the lowest in the series.

Table 1. Bond lengths obtained with the DFT-PBE method for the various crystal structures reported in Figure 2.

	Cu ₂ O	CuVO ₃	CuNbO ₃	$Cu_5Ta_{11}O_{30}$
Cu-O (Å)	1.85	2.01	1.81 / 1.87	1.86 / 1.88
M-O (Å)	-	1.79 / 2.06	1.80 / 2.12	1.97 / 2.04