Supporting Information:

Strong Optical Absorption in $CuTaN_2$ Nitride Delafossite

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Table S1. Refined atomic coordinates of $NaTaN_2$ and $CuTaN_2$.

Atoms	x	y	z
$NaTaN_2$			
Na	0	0	0.5
Ta	0	0	0
N	0	0	0.268
$CuTaN_2$			
Cu	0	0	0
Ta	0	0	0.5
N	0	0	0.19

Table S2: ΔH_f of $CuTaN_2$ in the 10 lowest energy crystal structures.

Structure	ΔH_f (eV/atom)	Structure	ΔH_f (eV/atom)
$AgFeO_2$	-0.665	$LiYO_2$	-0.597
$NaNiO_2$	-0.664	$CsGaS_2$	-0.597
$CaMnSb_2$	-0.627	$KFeS_2$	-0.597
$LiBO_2$	-0.599	$LiCsBr_2$	-0.597
$CuLaS_2$	-0.598	$NaBiO_2$	-0.596

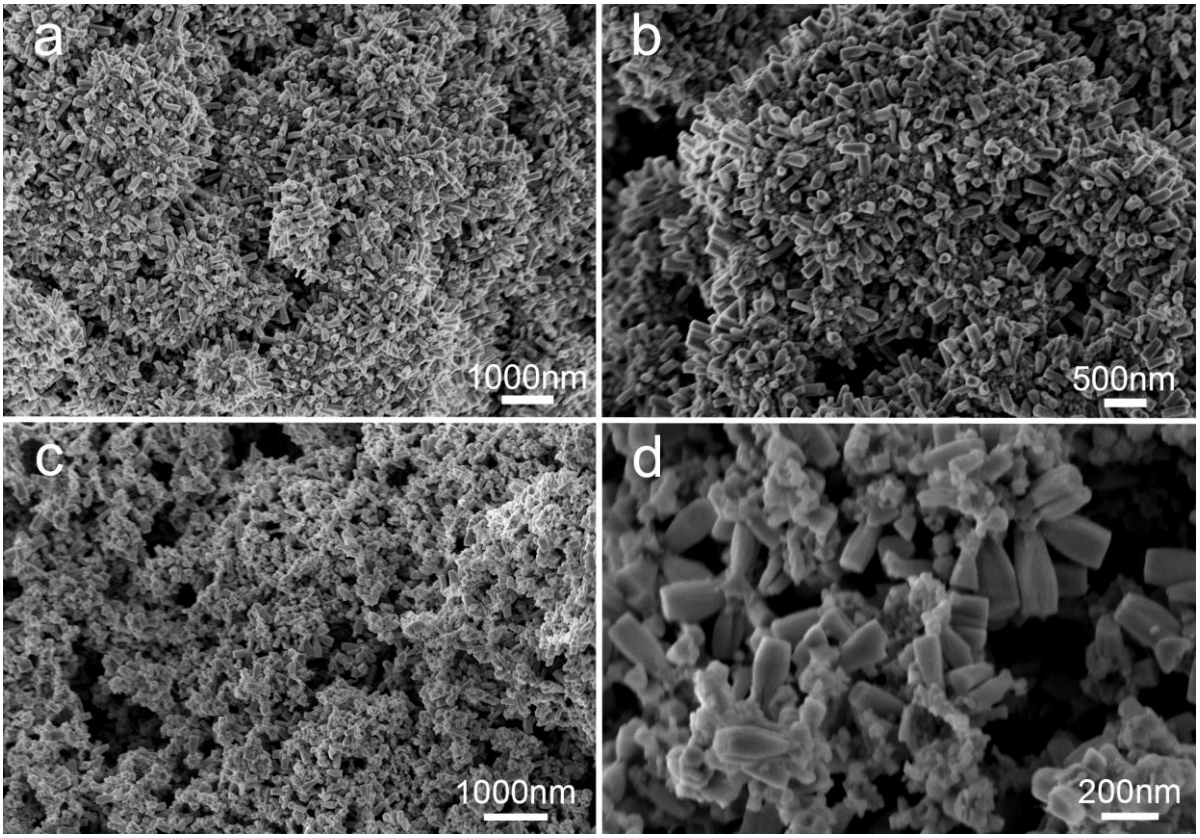

Figure S1. SEM images of (a, b)$NaTaN_2$ and (c, d) $CuTaN_2$

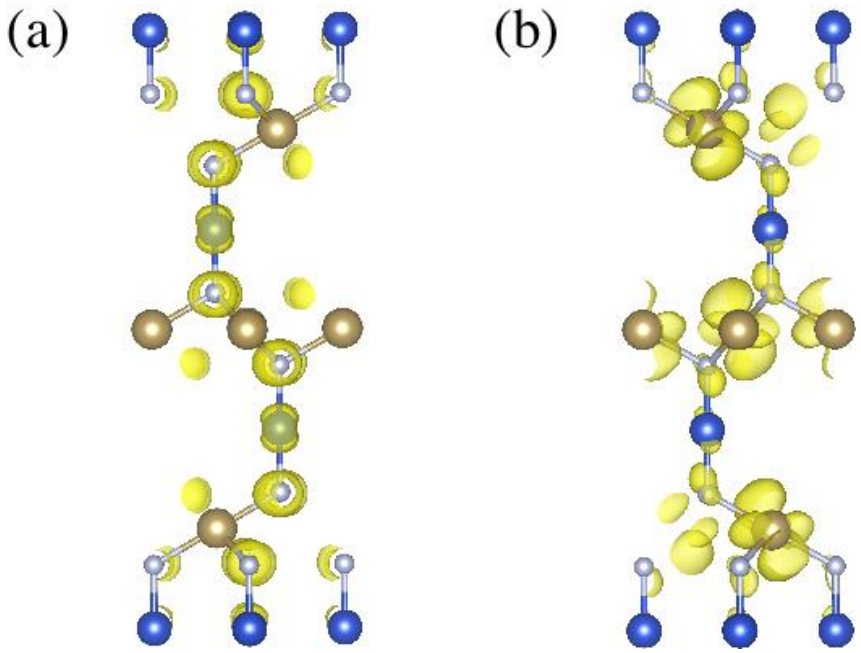

Figure S2. The electronic wave functions that correspond to the state at (a) the valence band maximum and (b) the conduction band minimum of $CuTaN_2$: Cu (blue), Ta (brown) and N (light blue)