

Supporting Information for

**CuTaS<sub>3</sub>: Intermetal *d-d* transitions enable high solar absorption**

Jaeseok Heo,<sup>†</sup> Liping Yu,<sup>‡,||</sup> Emmeline Altschul,<sup>†</sup> Benjamin E. Waters,<sup>§</sup> John F. Wager,<sup>§</sup> Alex Zunger,<sup>‡</sup>  
and Douglas A. Keszler\*,<sup>†</sup>

<sup>†</sup>Department of Chemistry, Oregon State University, Corvallis, Oregon 97331-4003 USA

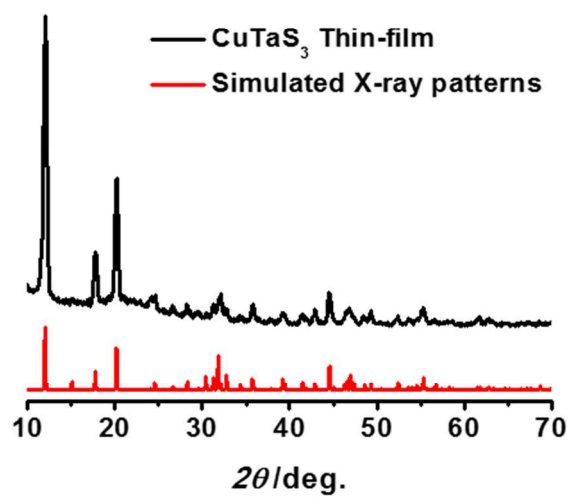
<sup>‡</sup>University of Colorado, Boulder, Colorado 80309, USA

<sup>||</sup>National Renewable Energy Laboratory, Golden, Colorado 80401, USA

<sup>§</sup>School of Electrical Engineering and Computer Science, Oregon State University, Corvallis, Oregon  
97331-5501, USA

**Table S1.** Refined atomic coordinates for CuTaS<sub>3</sub>.

Atoms	<i>x</i>	<i>y</i>	<i>z</i>
Cu	0.228064	0.75	0.21284
Ta	0.107494	0.25	0.36986
S1	0.076645	0.25	0.56685
S2	0.080781	0.25	0.5967
S3	0.27933	0.75	0.4028



**Figure S1.** X-ray diffraction pattern of CuTaS<sub>3</sub> thin-film. X-ray diffraction pattern simulated with single-crystal data of CuTaS<sub>3</sub>.