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Supplementary information

Earth-abundant Cu-based chalcogenide semiconductors as photovoltaic absorbers

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Table S1 Selected bond angles (°) for $Cu_3PS_{1.89}Se_{2.11}$ and $Cu_3PS_{0.71}Se_{3.29}$ (Q = S, Se).

	$Cu_3PS_{1.89}Se_{2.11}$	$Cu_3PS_{0.71}Se_{3.29}$
Q(1)-Cu(1)-Q(2)	113.25(6)	112.34(6)
Q(1)-Cu(1)-Q(3)	110.12(3)	110.53(4)
Q(2)-Cu(1)-Q(3)	107.94(4)	107.70(4)
Q(3)-Cu(1)-Q(3)	107.26(5)	107.88(6)
Q(1)-Cu(2)-Q(2)	108.37(4)	108.18(4)
Q(1)-Cu(2)-Q(3)	114.20(4)	113.70(4)
	103.51(4)	103.50(4)
Q(2)-Cu(2)-Q(3)	113.88(4)	114.39(5)
	110.57(4)	110.38(4)
Q(3)-Cu(2)-Q(3)	105.77(3)	106.11(3)
Q(1)-P-Q(2)	112.21(9)	112.22(10)
Q(1)-P-Q(3)	108.35(6)	108.17(8)
Q(2)-P-Q(3)	109.11(6)	109.27(9)
Q(3)-P-Q(3)	109.70(8)	109.73(10)

Table S2 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Cu_3PS_{1.89}Se_{2.11}$ and $Cu_3PS_{0.71}Se_{3.29}$ (Q = S, Se). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
			$Cu_3PS_{1.89}Se_{2.11}$			
Cu (1)	29(1)	25(1)	24(1)	2(1)	0	0
Cu (2)	27(1)	27(1)	23(1)	-1(1)	-1(1)	-1(1)
P	8(1)	8(1)	8(1)	1(1)	0	0
S (1)	13(1)	16(1)	10(1)	0(1)	0	0
Se (1)	13(1)	16(1)	10(1)	0(1)	0	0
S (2)	15(1)	12(1)	13(1)	-1(1)	0	0
Se (2)	15(1)	12(1)	13(1)	-1(1)	0	0
S (3)	12(1)	13(1)	13(1)	0(1)	-1(1)	-2(1)
Se (3)	12(1)	13(1)	13(1)	0(1)	-1(1)	-2(1)
			$Cu_3PS_{0.71}Se_{3.29}$			
Cu (1)	28(1)	25(1)	22(1)	3(1)	0	0
Cu (2)	28(1)	26(1)	20(1)	-1(1)	0(1)	-1(1)
P	10(1)	11(1)	6(1)	1(1)	0	0
S (1)	13(1)	17(1)	9(1)	0(1)	0	0
Se (1)	13(1)	17(1)	9(1)	0(1)	0	0
S (2)	15(1)	12(1)	13(1)	-1(1)	0	0
Se (2)	15(1)	12(1)	13(1)	-1(1)	0	0
S (3)	12(1)	13(1)	14(1)	0(1)	-1(1)	-2(1)
Se (3)	12(1)	13(1)	14(1)	0(1)	-1(1)	-2(1)