

# Exploiting XPS for the identification of sulfides and polysulfides. SUPPORTING INFORMATION

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## Tables

Table S.I.T1: Peak-fitting parameters of S<sup>2-</sup> determined on ground sulfide minerals (10 minutes under Argon)

		Binding Energy	FWHM	
Cu <sub>3</sub> AsS <sub>4</sub>	S2p <sub>3/2</sub>	161.8 (0.1)	1.4 (0.2)	
FeAsS	S2p <sub>3/2</sub>	162.1 (0.1)	1.5 (0.2)	
	SKLL	Kinetic Energy	FWHM	Area comp./Area <sup>1</sup> D
Cu <sub>3</sub> ASS <sub>4</sub>	<sup>1</sup> D SKLL	2116.0 (0.2)	1.6 (0.2)	1
	sat SKLL	2111.8 (0.2)	2.5 (0.1)	0.05
	<sup>1</sup> S SKLL	2107.8 (0.2)	2.5 (0.2)	0.1
FeAsS	<sup>1</sup> D SKLL	2116.4 (0.2)	1.4 (0.1)	1
	sat SKLL	2112.3 (0.2)	2.3 (0.2)	0.05
	<sup>1</sup> S SKLL	2108.2 (0.2)	2.3 (0.2)	0.1

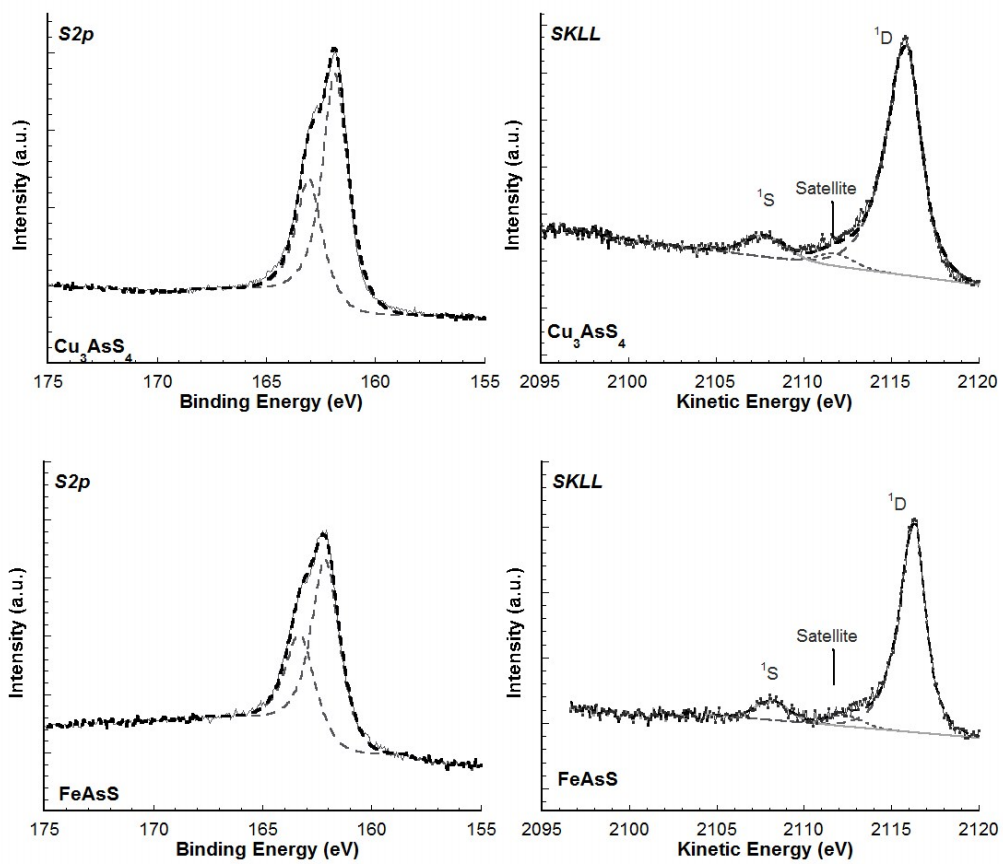
Table S.I. t2: XPS quantitative composition of the commercial alkali metal sulfides determined according to first principle method. Accuracy is estimated to be  $\pm 10$  at%

	Cation at%	Sulfur tot at%	S at% for each component
Li <sub>2</sub> S	66  (Li - S <sup>2-</sup> and Li - S <sub>n</sub> <sup>2-</sup> : 32.5%;  Li – sulfate and sulfite: 33.5%)	34	Sulfide 13%
			Terminal S 2%
			Central S 3%
			Sulfite 14
			Sulfate 2%
Na <sub>2</sub> S	40	60	Terminal S 18%
			Central S 37%
			Sulfate 5%
Na <sub>2</sub> S <sub>4</sub>	36	64	Terminal S 23%
			Central S 37%
			Sulfate 4%
K <sub>2</sub> S <sub>n</sub>	43	57	Terminal S 28%
			Central S 24%
			Sulfate 4%

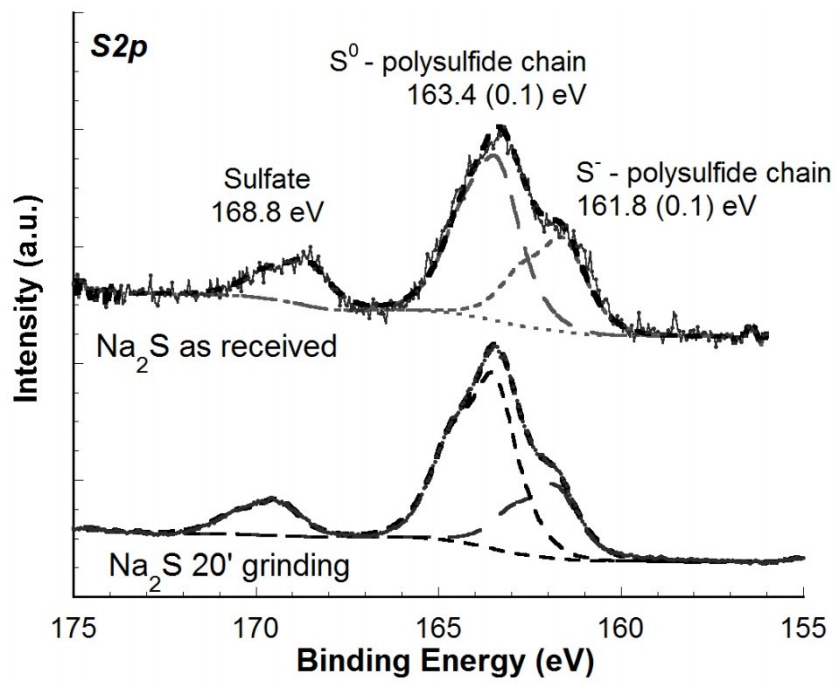
**Figure captions:**

S.I. Fig. 1: *S2p and SKLL spectra of ground sulfide minerals: enargite ( $\text{Cu}_3\text{AsS}_4$ ), chalcopyrite ( $\text{CuFeS}_2$ ) and arsenopyrite ( $\text{FeAsS}$ ).*

S.I. Fig. 2: *S2p spectra of as received  $\text{Na}_2\text{S}$  and of  $\text{Na}_2\text{S}$  after grinding (10 minutes) under Argon atmosphere (glove box).*



*S.I. Fig. 1*



S.I. Fig. 2