Structure and Electronic Properties of the Quasi-One-Dimensional $Ba_2Co_{1-x}Zn_xS_3$ Series

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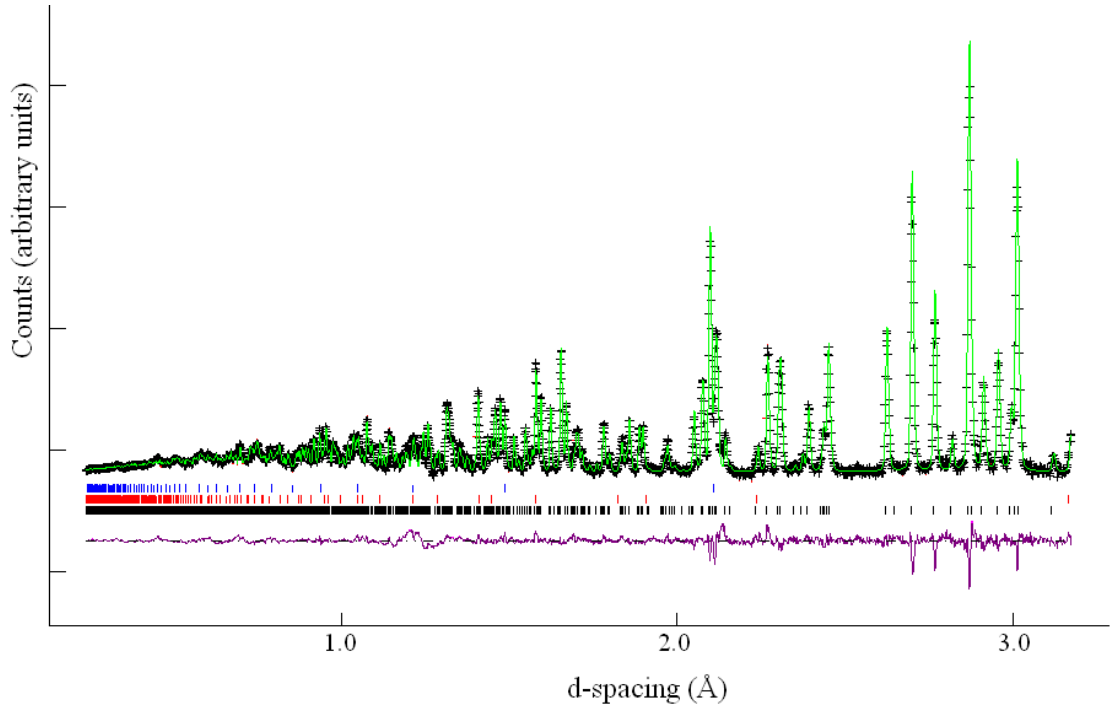

Figure S1 Rietveld refinement against neutron diffraction data for $Ba_2Co_{0.5}Zn_{0.5}S_3$: Black line (observed), green line (calculated) and purple line (difference). Black tick marks correspond to $Ba_2Co_{0.5}Zn_{0.5}S_3$, red to BaS and blue to the vanadium can.

Atom	x	y	z	U	F
Ba1	0.8264(2)	0.4812(1)	0.25	0.0041(3)	1
Ba2	0.4878(2)	0.6723(1)	0.25	0.0011(2)	1
Co	0.7484(2)	0.1986(2)	0.25	0.0002(3)	0.5
Zn	0.7484(2)	0.1986(2)	0.25	0.0002(3)	0.5
S1	0.8640(3)	0.0525(3)	0.25	0.0019(2)	1
S2	0.5594(2)	0.1421(3)	0.25	0.0028(2)	1
S3	0.2283(3)	0.7078(2)	0.25	0.0019(2)	1
$R_p = 2.42\%$		$R_{wp} = 1.45\%$		$\chi^2 = 3.94$	

Table S1 Atomic positions, thermal parameters and fractional occupancies for $Ba_2Co_{0.5}Zn_{0.5}S_3$

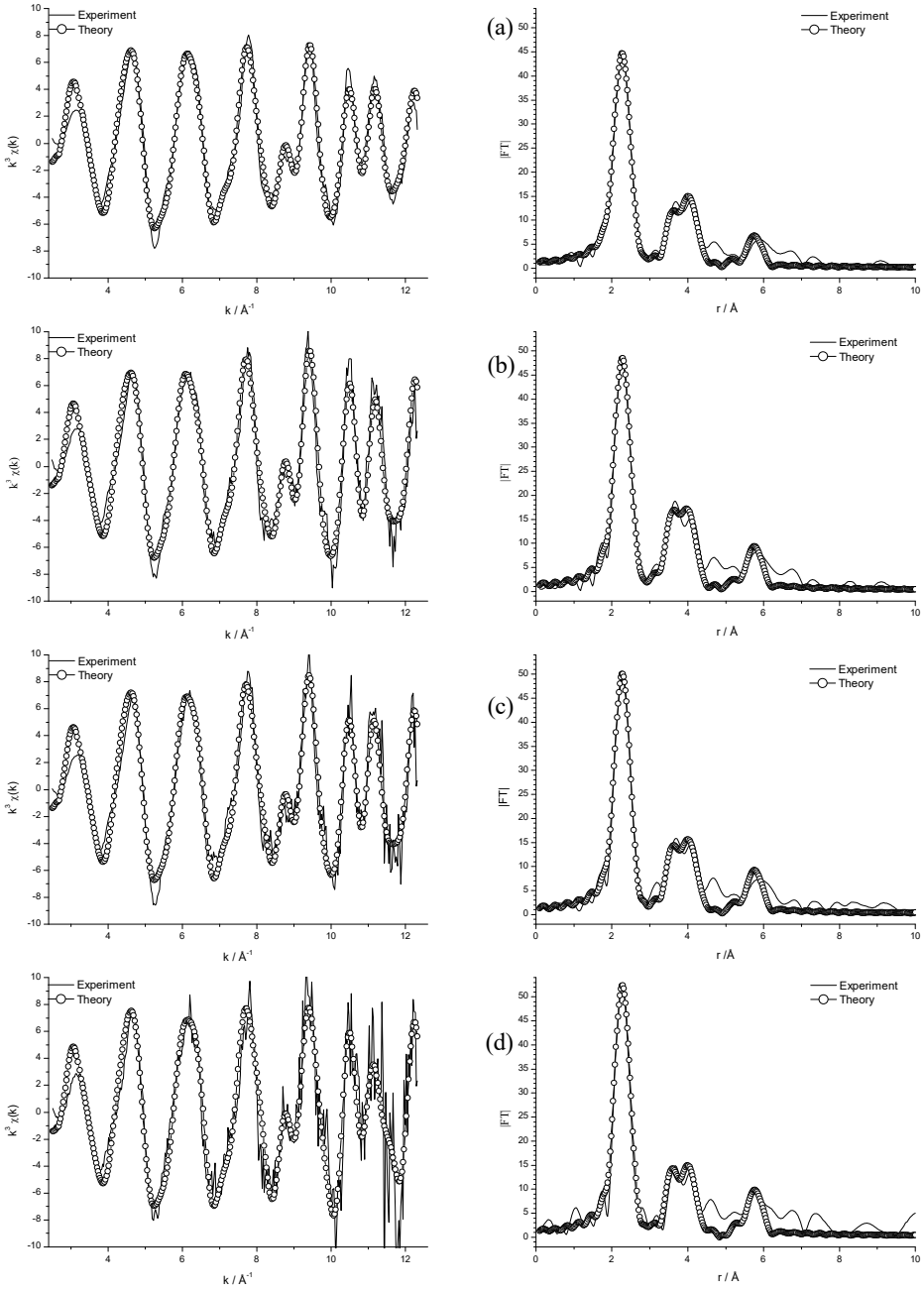

Figure S2 Co K-edge EXAFS (left) and FT (right) of (a) Ba_2CoS_3 (b) $Ba_2Co_{0.75}Zn_{0.25}S_3$ (c) $Ba_2Co_{0.5}Zn_{0.5}S_3$ and (d) $Ba_2Co_{0.25}Zn_{0.75}S_3$

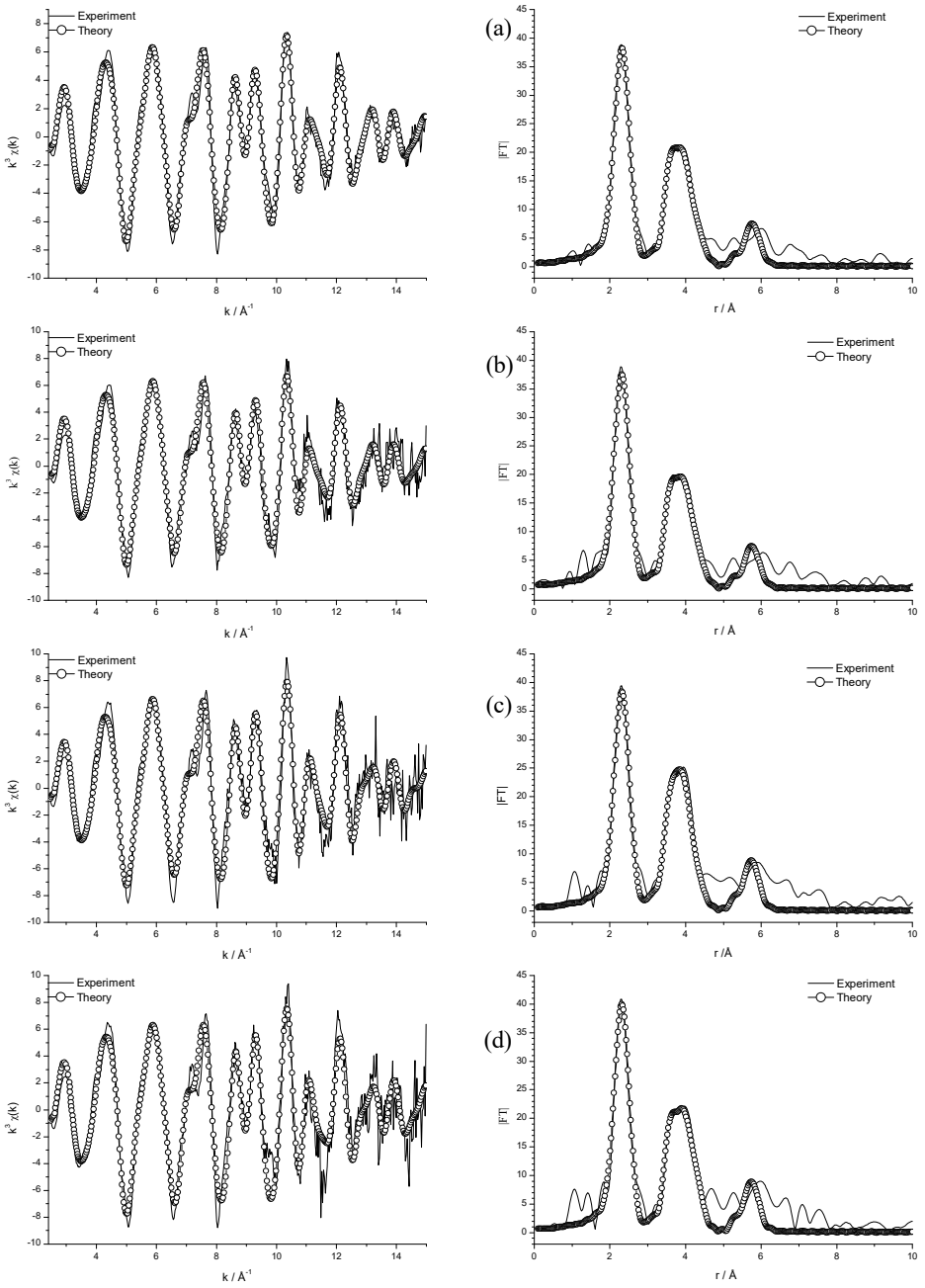

Figure S3 Zn K-edge EXAFS (left) and FT (right) of (a) Ba_2ZnS_3 (b) $Ba_2Co_{0.25}Zn_{0.75}S_3$ (c) $Ba_2Co_{0.5}Zn_{0.5}S_3$ and (d) $Ba_2Co_{0.75}Zn_{0.25}S_3$