Electronic Supplementary Information

Modelling polar wurtzite ZnS nanoparticles: the effect of sulphur supersaturation on size- and shape-dependent phase transformations

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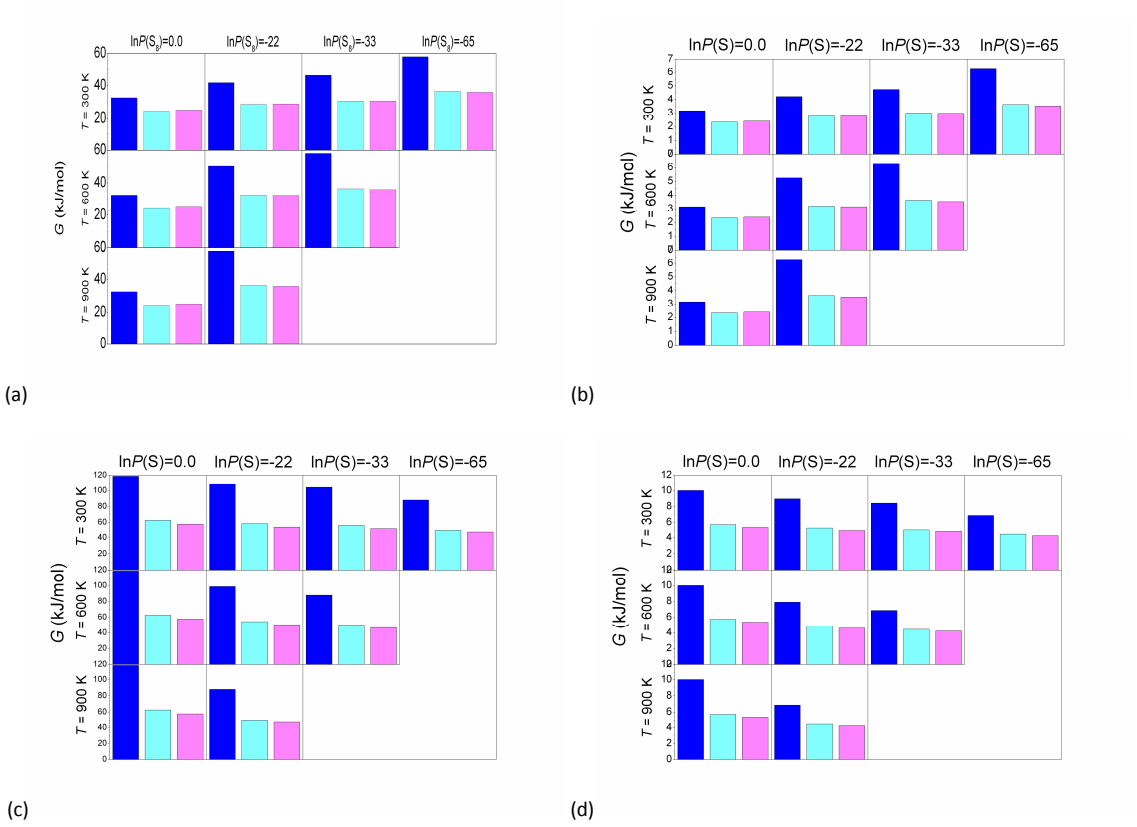

Fig. S1 - An initial sample of <*D*,*T*,*P*> space, taken by comparing the total free energies belonging to 5 nm (a and c) and 50 nm (b and d) shapes with S-terminated (a & b) and Zn-terminated (c & d) surfaces at nine different temperature/pressure points. Shapes are formed from {10-11} and {0002} (blue), {10-12}(cyan) and {10-13}(pink) surfaces. Truncation in the <0001> direction was optimised for each shape at each <*T*,*P*> point.

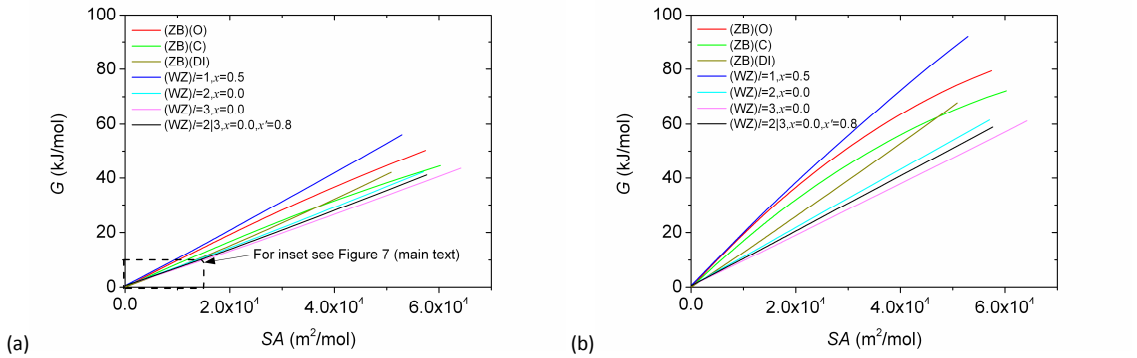

Fig. S2 – Total free energies of S-terminated WZ and ZB shapes under (a) S-rich and (b) Zn-rich conditions at 900 K. Inset in (a) shown in Fig. 7 of main article.

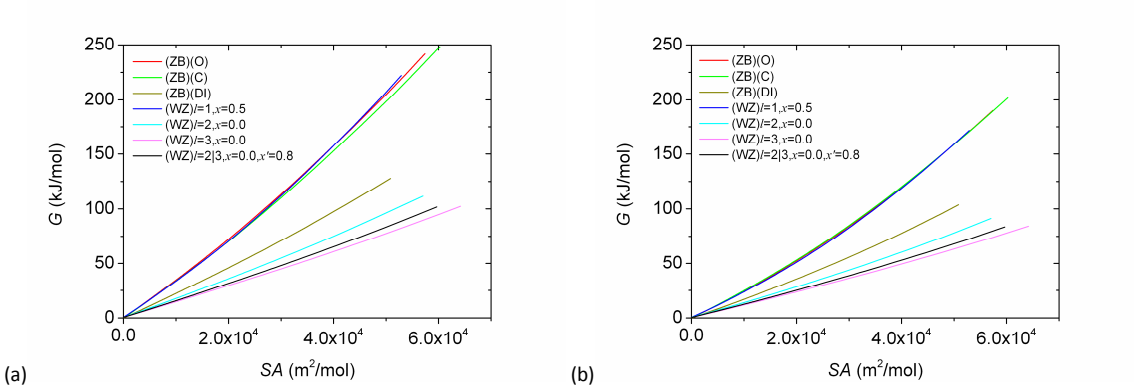

Fig. 3 – Total free energies of Zn-terminated WZ and ZB shapes under (a) S-rich and (b) Zn-rich conditions at 900 K.

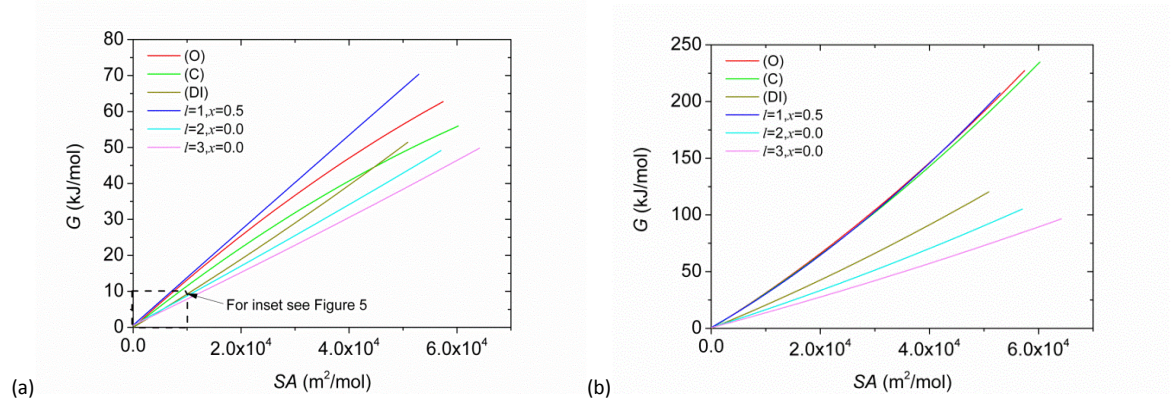

Fig. 4– Total free energies of (a) S-terminated and (b) Zn-terminated WZ and ZB shapes at a sulphur partial pressure lnP(S8)=-22 at 300 K.

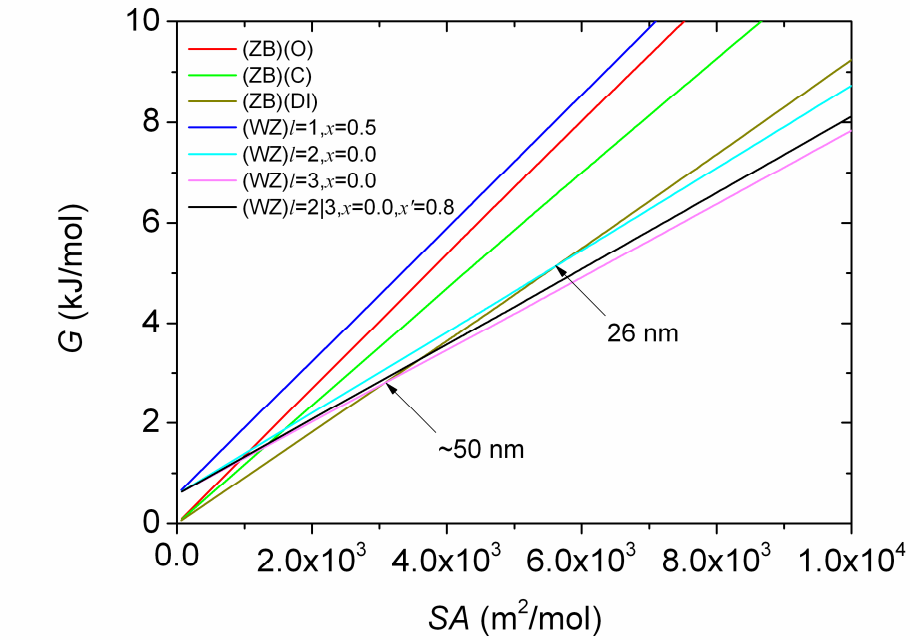

Fig. 5- Inset from Fig. 4(a) showing energetic crossovers between ZB and WZ shapes at 300 K.

Electronic Supplementary Material (ESI) for Journal of Materials Chemistry