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Simulation of the structure and stability of sphalerite (ZnS) surfaces

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ABSTRACT

Atomistic simulation techniques were used to investigate the surface energies and stabilities of the sphalerite form of ZnS. The results show that for pure ZnS the lowest energy surfaces are type I and all of the form {110} with a calculated surface energy of 0.65 J/m^2. In addition, we illustrate how type III surfaces, such as {$\overline{1}$11}, can be stabilized with respect to {110} by the introduction of point defects to the surface layer. Such defects lead to changes in stoichiometry and to the valence state of surface species. In general, the results suggest that for Zn-poor surface stoichiometries, the (111) surface becomes the most stable, whereas for Zn-rich compositions the ($\overline{1}$$\overline{1}$$\overline{1}$) is stabilized to the greatest extent.