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The surface morphology of $CuFeS_2$: A hybrid-exchange density functional study[1] VINCENT HUAIR-YU CHEN, Department of Physics, Imperial College London, London SW7 2AZ, United Kingdom, RUTH MARTINEZ CASADO, Department of Theoretical Condensed Matter Physics, Autonomous University of Madrid, 28049 Madrid, Spain, GIUSEPPE MALLIA, NICHOLAS HARRISON, Thomas Young Centre, Department of Chemistry, Imperial College London, London SW7 2AZ, United Kingdom — The surface morphology of $CuFeS_2$ has been determined using hybrid-exchange density functional theory calculations. The (110) surface is identified to be the most stable non-polar surface with a surface energy of 0.58 Jm^{-1}. The polar (112)/($\overline{1}\overline{1}2$) surface pair is shown to be remarkably stable and thermodynamically preferred to the (110) surface if certain defects are included. The stability of the polar (112)/($\overline{1}\overline{1}2$) surface pair is attributed to a combination of geometric and electronic mechanisms localised to the (112) surface which combine to neutralise the electrostatic dipole perpendicular to the surface. The former entails a partial reversal of the surface atomic layer sequence while the latter involves dispersion of charge from the subsurface anions to neighbouring cations. Because of its stability, (112) and ($\overline{1}\overline{1}2$) facets always form a significant portion of the Wulff construction regardless of the growth conditions.

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