Goldschmidt 2023 Abstract
https://doi.org/10.7185/gold2023.18570

Modelling Morphology and Surface Speciation of Nanoparticles

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Any interfacial properties of minerals and minerals used in technological applications are affected by their surface composition and morphology, and these ultimately affect the surrounding environment. Here, a thermodynamic strategy to define a nanoparticle's morphology is coupled with ab initio data derived using density functional theory calculations. This allows us to link the atom-scale to the nano-scale and beyond, to predict the most thermodynamically stable particle' morphology based on the surface free energies of adsorbed surfaces as a function of temperature and partial pressures of the adsorbed species. Firstly, we provide insights into surface composition and determine the temperature of desorption of different adsorbed species. Secondly, we investigate multiple surfaces and determine the ratio between the different surfaces at conditions of temperature and pressure appropriate for the process under investigation. Finally, we bring the two together to evaluate morphology phase diagrams in the same fashion as three-component phase diagrams are built.