Nanoparticle structure, surface structure and crystal chemistry

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There is now good evidence that mineralogical nanoparticles have different chemical properties than their bulk analogs [1]. As much of the reactive properties of a phase are determined by its interface structure and chemistry, this suggests that nanoparticles may have quite different surfaces than larger crystallites. We are thus interested in determining nanoparticle surface structure, with the goal of eventually predicting it, and for this we require an understanding of the factors controlling surface atom arrangement.

Crystal chemical rules have been popular since Pauling's developments early in the 20th century, and are used today in interpreting structure-property relationships of extended crystals. However work by Gibbs and co-workers [2], and explanations developed by Burdette and others [3], demonstrate that the rules are consequences of molecular orbital interactions. This allows small molecular simulations to be applied to extended structures with remarkable validity.

In this talk we will examine what application of crystal chemical rules predicts about nanoparticle and bulk mineral surfaces, and where other important factors, such as electron confinement, may be significant. Examples will include nanoscale ZnS [4], goethite (α-FeOOH) [1], hematite (α-Fe_2O_3) [5], and TiO_2.

In addition we will discuss the factors controlling abundances of reactive nanoparticles on Earth's surface, and the type of effects they may have on chemical processes by virtue of their distinct properties.

References

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