

Effect of hydration layers and magnetic transitions on the stability of Fe-oxide nanoparticles

N.L. ROSS^{1*}, E.C. SPENCER¹, B.F. WOODFIELD² AND A.I. KOLESNIKOV³

¹VirginiaTech, Blacksburg, VA 24061, USA

(*correspondence: nross@vt.edu)

²Brigham Young University, Provo, UT 84602, USA

³ORNL, Oak Ridge, TN 37831, USA

Surface water on metal-oxide nanomaterials has become a topic of great interest in geochemistry as the stability of metal oxide materials at the nanoscale is provided, in part, by the occurrence of water confined to their surfaces. In this presentation, the thermodynamic properties of hydrated α -Fe₂O₃ (hematite) and Fe₃O₄ (magnetite) nanoparticles have been evaluated using inelastic neutron scattering (INS) spectroscopy. Inelastic neutron scattering (INS) provides key information about the structure and dynamics of the water species confined to the oxide surfaces. The complexity inherent in the structure of the nanoparticle hydration layers is reflected in their vibrational density of states (VDOS) from which their thermodynamic properties may be determined. We find that water confined on the surface of α -Fe₂O₃ nanoparticles has an isobaric heat capacity that exceeds that of ice-Ih at temperatures > 75 K, whereas the heat capacity for water on Fe₃O₄ is greater than that for ice-Ih at all temperatures. This is a consequence of the differing distribution of the librational modes of the two confined water systems. As neutrons have a magnetic moment they also provide a probe of the magnetic properties of nanoparticles. We observe both dispersed and non-dispersed magnetic signals in α -Fe₂O₃. We shall show how these magnetic transitions, coupled with the hydration layers, contribute to the overall stability of the α -Fe₂O₃ nanoparticles relative to Fe₃O₄.