TORI Z. FORBES,* SARA E. MASON,* JENNIFER BJORKLUND

Department of Chemistry, University of Iowa, Iowa City, IA 52242, * correspondence: tori-forbes@uiowa.edu, sara-mason@uiowa.edu

Small (1-2 nm) aluminum oxyhydroxide nanoparticles are of interest to geochemists because they are key to mineral paragenesis and possess highly reactive surfaces that can readily adsorb a range of contaminants. Previous work by Alexandra Navrotsky demonstrated that Kegin-type clusters containing 13 Al^{3+} cations (Al_{13}) are an important intermediate phase in the formation pathway of aluminum hydroxide precursors [1]. Additional studies indicated that heterometallic clusters, $GaAl_{12}$ and $GeAl_{12}$, possess slightly higher enthalpies of formation than the pure aluminum oxyhydroxide nanoparticles and also exhibit subtle differences in reactivity.[2 - 4] Building upon these previous studies, we are exploring bonding and energetics in these systems by combining experimental and computational methodologies. Our initial experiments suggest that there are subtle differences in the bonding that may influence the overall reactivity of the clusters and influence how the surface interacts with counter ions present in solution.

[1] Armstrong, Casey & Navrotsky (2011), *Proceedings of the National Academy of Sciences* 108, 14775-14779.

[2] Reusser, Casey & Navrotsky (2014), *American Mineralogist* 99, 2337-2342.

[3] Reusser, Casey & Navrotsky (2015), *Angewandte Chemie, International Edition* 54, 9253-9256.

[4] Stewart, Trudell, Alam, Ohlin, Lawler, Casey, Jett, & Nyman (2009), *Environmental Science & Technology*, 43, 5416-5422.