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Regression based analysis of factors controlling the formation of synthetic aluminosilicate nanoparticles

FAISAL T ADAMS[1], MCNEILL BAUER[1], CLEMENT LEVARD[2] AND F. MARC MICHEL[1]

[1]Virginia Tech

[2]CEREGE, Aix Marseille Univ, CNRS, IRD, INRA

Presenting Author: fadams@vt.edu

Synthetic nanoparticles composed of earth-abundant elements are highly reactive and can be produced using less resource-intensive methods, such as sol-gel synthesis. Among these, alumino(silicate) nanominerals, including imogolite nanotubes, are particularly noteworthy, with applications spanning sensing, catalysis, carbon sequestration, and drug delivery. However, the promise of technological uses of imogolite in applications is limited by the ability to synthesize pure phases at scale. This work investigates the complex interplay of physicochemical conditions that influence the formation and relative distribution of these particles, addressing questions that have been unresolved until now.

Nanoparticle products were synthesized and analyzed by powder X-ray diffraction, *in situ* and *ex situ* small-angle X-ray scattering, and transmission electron microscopy. Quantitative and semi-quantitative regression analyses were performed on phase abundances derived from linear combination fitting of powder diffraction patterns as a function of initial Al, Si, and OH concentrations and ratios, and the rate of OH addition. The resulting models show that the amount of OH added exerts the strongest control on precursor particle size and subsequently on the phase distribution of the final nanoparticle products, with Al concentration being the next most crucial factor. In the case of imogolite nanotubes, increasing concentration, and either high or low OH amounts, limit nanotube formation. The confidence levels were >99% for all linear regression models and explained up to 85% of the data variance for imogolite. This work also presents phase maps that delineate the synthesis space for this system of nanoparticles and extrapolates beyond the input conditions used here, while agreeing with results from other experimental studies. The methods developed from this study can be applied to understand complex chemical systems with competing influences and provide an approach for maximizing individual nanomaterial phase occurrence or produce controlled mixtures of nanoparticle phase products.