



Rising Stars

New Entrants

Country Profiles

About Science Watch

Methodology

Archives

Contact Us

**RSS** Feeds

The nanogoethite data is new, and data on metal uptake suggests

SW: Does it describe a new discovery, methodology, or synthesis of knowledge?

early growth. Finally, the paper describes how nanosized natural mineral phases may differ substantially

that the more disordered structures of the smaller particles alter the precise nature of binding to these nanoparticles compared to larger sized particles.

# SW: Would you summarize the significance of your paper in layman's terms?

in properties from their bulk analogs.

Natural nanoparticles, especially of reactive compositions such as iron oxides and hydroxides, may play a disproportionally important role in contaminant transport and sequestration in the environment. This is due to structural and chemical variations in the nanoparticles at very small sizes (0-20 nm) that are fundamentally different from larger crystallites and mineral surfaces, and to the incorporation of contaminants into nanoparticles during aggregation.



Figure 1

It is also shown that aggregation itself may be an important aspect of early nanoparticle growth, in competition with classical growth in an "atom by atom" mode. These considerations suggest that metal or anion contaminant transport (e.g. of arsenic, mercury, or copper) may be markedly changed if reactive nanoparticles are present or forming in the same environmental systems.

# SW: How did you become involved in this research and were any particular problems encountered along the way?

We have an interactive group of principal investigators at UC Berkeley and at Lawrence Berkeley National Laboratory who collaborate on nanoscience projects. We call our laboratory the "Berkeley Nanogeoscience Center" and investigations focus on the properties and reactivity of naturally occurring nanoparticles.

## SW: Where do you see your research leading in the future?

One of our main aims is to interpret the atomic-scale structural aspects of natural nanoparticles, especially at the surfaces, which give rise to altered reactivity and physical properties. This is an important research area in all of nanoscience, except that most engineered nanoparticles have surfaces terminated by capping ligands, and are generally well-defined.

With natural nanoparticles, the surfaces are not capped and vary with degree of crystallinity and growth conditions, and hence present a rich and variable field of reactive sites for interactions with natural agents, such as contaminants.

Study of this inherent complexity could lead to improved synthetic preparations of nanoparticles with precisely tuned properties, in chemical coherence with the natural environment. We have also found, and are continuing to study, the dramatic changes in water structure at nanoparticle surfaces observed in simulations.

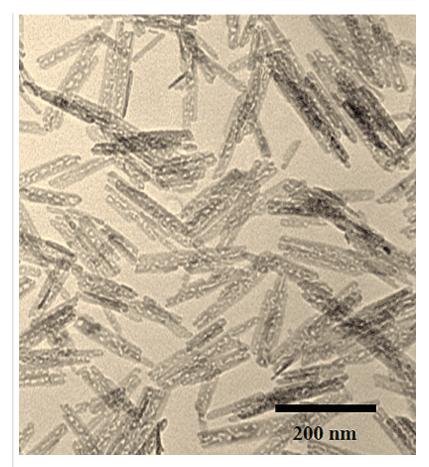
#### SW: Do you foresee any social or political implications for your research?

Tuned nanoparticle structure, and thus properties, may be very important in environmental remediation efforts. Efforts now underway to develop large-scale carbon sequestration methodology may also involve very specialized mineral nanoparticles to react with and precipitate high CO<sub>2</sub> brine solutions. These

types of applications can have potentially great social and political implications.

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#### Figure 1:



## Figure 1:

Nanogoethite particles formed from solution showing internal structural variations consistent with formation from smaller nanoparticles (about 5 nm diameters) via a process called oriented aggregation or OA. In this form of aggregation, the crystallites assemble with consistent crystallographic orientations to form a new larger single crystal. This type of formation process appears to compete with classical "layer by layer" growth in some cases, and leads to changes in the kinetics of growth in the nanoparticle size regime. During OA, or during aggregation without specific orientation, contaminants in the growth solution can be internally captured by the growing nanoparticles. Such encapsulation allows distant transport of contaminants compared to ordinary sorption processes. Photo by Christopher Kim (Chapman University). Taken at the National Center for Electron Microscopy (NCEM) LBNL.

KEYWORDS: HYDROUS FERRIC-OXIDE; MOLECULAR-DYNAMICS SIMULATIONS; ANOMALOUS LATTICE EXPANSION; PHASE-TRANSFORMATION; SURFACE COMPLEXATION; HEMATITE NANOPARTICLES; ORIENTED AGGREGATION; CRYSTAL-GROWTH; FERRIHYDRITE; SORPTION.

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