

Data Management Plan

The proposed research will generate detailed biogeochemical data from the combined batch experiments and molecular scale characterization. This data management plan will ensure the proper collection, analysis, storage, and dissemination of these data.

Data collection and analysis

Laboratory data (e.g., images, kinetic data, and spectra) collected during experiments will be recorded in laboratory notebooks or as computer files. Data collected at user facilities (e.g., XRD, SEM, TEM, and synchrotron light source) will be given descriptive file names and accompanied with a descriptive file, such as the sample nature, data collection condition, and problems encountered. Detailed experimental procedures will always be recorded. Reproducible experimental protocols, analytical techniques, and instrumental operation guidelines will be compiled as electronic standard operation protocols (SOP).

Data storage and format

Laboratory data and notebooks will be labelled and organized during and after the experiment. Files and notebooks within the same category (e.g. SEM data and synchrotron XAS data) will be grouped and archived based on experimental date. For data collected on special instruments, they will be stored in both original and universal format (e.g., ascii file, .jpg image). A descriptive file will always accompany the data folder to describe the experimental nature, such as operator, date, time, location, instrumentation, methods, and special notes.

Designated notebooks for each user facility data collection will be organized and stored in the laboratory or by the PI. Computer files will be stored on laboratory computers and shared using cloud-based servers such as Dropbox or Google Documents among the research teams. At Georgia Tech, all computer files will be regularly backed up on a SharePoint Georgia Tech server.

Dissemination of data

All the results will be disseminated to the scientific community through publications at high-profile peer-reviewed journals and through presentations at scientific conferences, as well as on the web pages of the involved laboratories. Experimental data sets underlying results reported in publications will be included as on-line Supporting Information for publications, thereby guaranteeing long-term archiving and widespread accessibility to the scientific community, as well as encouraging further developments in the scientific interpretation and use of the data.