

## Microbial Fe, Mn & As redox transformations and their contributions to As removal from drinking water in household sand filters in Vietnam

ANDREAS KAPPLER<sup>1\*</sup>, KATJA NITZSCHE<sup>1</sup>, ANKITA BHANSALI<sup>1</sup>,  
MICHAEL BERG<sup>2</sup>, PHAM THI KIM TRANG<sup>3</sup>, PHAM HUNG VIET<sup>3</sup>,  
SEBASTIAN BEHRENS<sup>1</sup>

<sup>1</sup>Geomicrobiology Group, University of Tuebingen, Germany,  
andreas.kappler@uni-tuebingen.de (\*presenting author)

<sup>2</sup>Eawag, Swiss Federal Institute of Aquatic Science and Technology,  
Dübendorf, Switzerland

<sup>3</sup>Center for Environmental Technology and Sustainable Development  
(CETASD), Hanoi University of Science

Worldwide more than 100 million people ingest detrimental concentrations of arsenic by consuming groundwater contaminated from natural geogenic sources. Many Asian countries, in particular Vietnam, Bangladesh, India, and Cambodia are known to be affected by high groundwater arsenic concentrations as a result of reducing aquifer conditions [1]. Household sand filters are simple to operate and remove most of the arsenic from the groundwater containing arsenic and ferrous iron with an iron/arsenic ratio of at least 50 leading to As values of <50 or even <10 µg/L [2]. The installation and operation costs of household sand filters are low and the construction materials are locally available. The filters can treat a reasonable amount of groundwater within a short time and they are easily installed by the affected communities. Oxidation of dissolved iron present in the groundwater leads to the formation of sparsely soluble iron (oxyhydr)oxide particles in the sand filters, which bind negatively charged and neutral arsenic species and reduce arsenic concentrations in the water [2, 3].

Although household sand filters are an effective technical solution for mitigating arsenic exposure, not much is known about microbial iron, manganese, and arsenic redox transformations occurring in the filters and their effect on filter efficiency. Therefore, one of the goals of this study was to isolate, identify, and quantify Fe, Mn, and As-oxidizing and -reducing microorganisms from a arsenic removal sand filter and to study their specific Fe, Mn, and As redox activities. Water samples and filter solids were collected from a local sand filter close to the city of Hanoi, Vietnam. The samples were geochemically and mineralogically characterized. Total iron, arsenic, manganese, and phosphate concentrations, pH, TOC, TIC measurements, as well as total cell counts were performed on samples from various depths of the sand filter. Most probable number counts confirmed the presence and activity of various iron, manganese, arsenic redox-processes and their distribution within the water filter. This research aims to better understand the microbial redox transformation processes that drive arsenic/manganese/iron mineral interactions in household sand filters and to give recommendations for improved filter use and filter material disposal.

[1] Winkel *et al.* (2008) *Nature Geosci.* **1**, 536-542. [2] Berg *et al.* (2006) *Environ. Sci. Technol.* **40**, 5567-5573. [3] Kleinert *et al.* (2011) *Environ. Sci. Technol.* **45**, 7533-7541.

## First principles study of the structure and compressibility of MgSiO<sub>3</sub> glass

DIPTA GHOSH<sup>1</sup>, BIJAYA KARKI<sup>1\*</sup> AND LARS STIXRUDE<sup>2</sup>

<sup>1</sup>Louisiana State University, Baton Rouge, USA, dghosh2@lsu.edu,  
karki@csc.lsu.edu (\* presenting author)

<sup>2</sup>University College London, London, UK, l.stixrude@ucl.ac.uk

Silicate glasses have been widely studied because they are considered as analog of geologically relevant silicate melts. Experimental studies have suggested that silicate glasses undergo significant structural changes including irreversibility under compression. Here, we report first-principles molecular dynamics study of the equation of state and structure of MgSiO<sub>3</sub> glass at 300 K as a function of pressure. Our simulations show that the glass at ambient condition is composed of primarily Si-O tetrahedra (with ~95% abundance, the mean coordination number being ≥ 4), which are partially linked with each other via bridging oxygens (present in 35%, the remaining being non-bridging oxygens). As pressure increases, the mean Si-O coordination gradually increases to 6 occurring through the increased appearance of five-fold (pentahedral) states at low pressure and then six-fold (octahedral) states at high pressure. On the other hand, Mg-O coordination, which is a mixture of four-, five- and six-fold species at zero pressure, picks up more high-coordination (seven- to nine-fold) species on compression and its mean value increases from 4.5 to 8 over the pressure range studied. Consistently, the anion-cation coordination increases under pressure with the appearance of oxygen triclusters (O atoms coordinated with 3 Si or 3 Mg atoms) and the mean O-Si (O-Mg) coordination eventually reaching (exceeding) 2. We find that glass densification is rather rapid initially and becomes more gradual at pressures above 20 GPa. This behavior can be associated with the way the glass structure changes in terms of bond distances, bond angles and coordination environments as pressure increases. On decompression, the system fails to revert back to its initial structural state, consistent with the experimental observations, and this irreversibility can be attributed to the memory effects, i.e., to continuing existence of high coordination species (pentahedra and octahedra) to larger volumes.