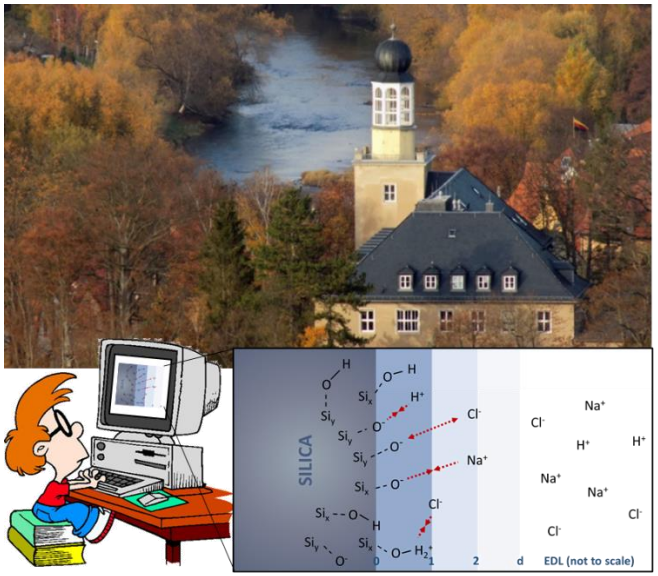
WORKSHOP IN GEOCHEMICAL MODELLING WITH PYTHON AND COMSOL

25th and 26th November 2021

FSU Jena, Germany

– Hybrid format –



Organized by:

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Background:

Surface chemistry of mineral phases in aqueous environments is a broad topic of interest in many fields including colloidal stability, element sorption and transport in nanoconfined systems. This characteristic physical-chemical interfacial behaviour has a wide range of applications in industrial, biological, and environmental systems including water treatment, radionuclide migration from radioactive waste disposal areas, workability of cementitious materials, among others. Surface chemistry can be accounted for by experimental approaches (e.g., force-distance measurements, electrokinetic analyses) or through calculations with different spatial and temporal resolutions (e.g., Molecular Dynamics, Surface Complexation Models, Reactive Transport Modelling).

A free-access code named SINFONIA (Speciation and INter-particle FOrces for Nanoscale InterActions) has been recently published (Gil-Díaz et al. 2021), implemented in Python and COMSOL. This code accounts for solid/liquid electrostatic interactions with state-of-the-art surface complexation models through charge regulation, i.e., considering solution and surface speciation changes upon particle approach. Overall, the code allows quantifying consistently aqueous chemistry and surface complexation models for various geometries, including chemo-mechanical interactions between equal and unequal surfaces for arbitrary electrolytes. This code presents some advantages regarding other commercial software (e.g., PHREEQC, MINTEQ, etc.) and a large variety of potential applications accounting from colloidal suspensions to new possibilities to assess the chemistry in nano-confined systems.

Scope:

The aim of this workshop is to provide basic knowledge on surface complexation modeling and to promote the use of SINFONIA, including:

1. Explanation of the current knowledge on surface chemistry of single and interacting surfaces, developed forces between surfaces and implications between the coupling of chemical and mechanical processes.
2. The use of SINFONIA (installation and code description).
3. Applications/exercises in Python and COMSOL
4. View on experimental approaches with a laboratory tour at IGW FSU Jena.
5. Overview of further applications of the code for 2D geometries

Workshop format:

The workshop will take place in a hybrid format. Online participation is free and unlimited in the number of participants. Onsite participants will adhere to the 3G rule and will be limited to 15 people.

Lab visit:

For onsite participants, a short visit to the laboratory installations in IGW Burgweg 11 is foreseen.

Target audience:

Geochemists, chemists, biologists, civil engineers, or material scientists, familiar with AFM, surface force apparatus, or electrokinetic measurements, or simply interested in chemical speciation and nanopore speciation. Not limited to FSU members. Basic knowledge of Python and COMSOL are useful. All attendees onsite should bring their own laptops.

Agenda:

25th November 2021	
8:45 – 9:00	Arrival time for onsite and online (zoom) attendees
9:00 – 9:15	Welcome and introduction to the workshop
9:15 – 10:15	Theory of surface complexation models and DLVO
20 min break	
10:35 – 12:00	Introduction to SINFONIA-for-One (setting up a simple example)
60 min break	
13:00 – 15:00	Case study 1: sorption at equal surfaces + force-distance curves
20 min break	
15:00 – 17:00	Case study 2: bidentate sorption at equal surfaces
26th November 2021	
8:45 – 9:00	Arrival time for onsite and online (zoom) attendees
9:00 – 10:00	Basics of calculations in interstitial solutions and chemo-mechanical coupling
20 min break	
10:20 – 12:00	Case study 3: interstitial profiles and chemo-mechanical coupling
60 min break	
13:00 – 15:00	Case study 4: sorption at unequal surfaces
15:00 – 15:45	Invited guest speaker (online): Beyond SINFONIA, SCM for uneven and heterogeneous surfaces applied for 2D geometries (Dr. Frank Heberling, INE-KIT)
15:45 – 16:00	Closing the event
16:00 – 17:00	Lab tour IGW-FSU for onsite attendees

Preliminary location for onsite workshop:

Thursday 25th Nov.: Carl-Zeiss-Str. 3
Friday 26th Nov.: Burgweg 11

Enrolling and registration fees:

Participation is free of charge. For organizational purposes, participants should register **before the 15th November 2021** by filling in the **Registration Form** and sending it via email to the organizing committee. More information (e.g., zoom link and lecture materials) will be communicated via email.