International Symposium 2025
Molecular modeling in soil science – achievements and perspectives

September 24, 2025 - September 26, 2025

CECAM-AT

Organizing committee:

BOKU University, Vienna, Austria

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Martin Gerzabek - *Institute of Soil Science*

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1. Description

It is undeniable the major role of soils in ecosystem functions at very different spatial and temporal scales (local and global) from microscopic to macroscopic phenomena. Soil plays a fundamental role as sink and source of gases being part of the greenhouse effect and thus in the fight against climate change. Soil serves as an ecological buffer for numerous chemical species such as contaminants and fertilizers and is a major factor in the global hydrological cycle. The exchange of energy and mass takes places at the interface, where physical, chemical and biological processes determine their fate. Moreover, soil is a substrate that provides sustenance and nutrients to plants, microorganisms and higher organisms.

In view of the great demand for information regarding best practices for soil use and management, as well as remediation, new methods traditionally used in other areas have come into play to provide a better understanding of important soil processes and functions. With the arrival of powerful and more efficient computers, molecular modeling has become an important tool, offering insights into scales unattainable experimentally, being able to simulate complex molecular systems. The application of such methods in soil science has proven success to understand the interactions within soil at microscopic level, key to determine the fate of pollutants.

Following up the symposia organized in 2005 and 2009, this symposium represents an opportunity to bring together scientists of high prestige in different areas of molecular modeling applied to soil science to discuss the state-of-the-art, promote meaningful discussions and contrast in-depth points of view to determine future perspectives and challenges regarding molecular modeling applied to soil science. Furthermore, the symposium presents an opportunity to foster cooperation and dissemination of knowledge on methods for the simulation of representative soil models, according to today's needs as well as the prediction of physicochemical properties.

All participants will enjoy a pleasant atmosphere surrounded by other experts in fields of soil science. Molecular modeling methods applied to various areas in soil science will be covered but not limited. The symposium is open for the presentation of experimental techniques combined with molecular modeling studies such as the contributions in the field of microcalorimetry, Nano-SIMS, AFM, XANES and similar techniques. These will be divided into plenary sessions:

- Advances of MM methods in soil science
- Soil minerals
- Soil organic matter (SOM)
- Interactions of minerals and SOM
- Fate of contaminants in soils

During the three days of the symposium, there will be talks by experts, oral presentations and poster sessions to share the most recent advances in each field. On the second day, a mini workshop to build SOM models using the Vienna Soil Organic Matter Modeler (VSOMM) tool will be held in place.

The symposium will take place at the BOKU University, leader in the fields of life sciences in Europe and distinguished by its holistic and sustainability-based approach to research and teaching, located in the city of Vienna, renowned for its rich cultural heritage, stunning architecture, and vibrant arts scene.

Key References

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2. Program

Wednesday, September 24th 2025

13.00 – 14.00 Lunch snacks

13.50 – 14.00 Hunting horn group of BOKU University "Gregor Mendel"

14.00 – 14:30 Opening: Welcome & Introduction

14:00 - 14:10	Rector Eva Schulev-Steindl, Rector of BOKU University
14:10 - 14:20	Sophie Zechmeister-Boltenstern, Head of the Institute of Soil Research, BOKU University
14:20 - 14:30	Andreas Baumgarten, President of the Austrian Soil Science Society (ÖBG)

14.30 – 16.15 Advances of MM methods in soil science (Chair: Martin Gerzabek)

14:30 - 15:15	Edgar Galicia-Andrés *Impact of computer simulations in soil science*
15:15 - 15:45	Hessam Yazdani *Computational perspectives on soil interface phenomena: strength, ion transport, and PFAS retention*
15:45 - 16:15	Hannah Pollak *ClayCode: A Python toolkit for modelling realistic clay systems*

16.15 – 16.45 Coffee break

16.45 – 17.45 Advances of MM methods in soil science (Chair: Chris Oostenbrink)

16:45 - 17:15	Milan Předota *Characterization of solid/liquid interfaces by computational nonlinear optical spectroscopy*
17:15 - 17:45	Sébastien Le Crom *The role of explicit polarizability in molecular modeling of clay-water interfaces across hydration states*

17.45 Posters, wine and bread

Thursday, September 25th 2025

9.00 – 10.45 Soil minerals (Chair: Martin Gerzabek)

9:00 - 9:45	Andrey Kalinichev *Recent advances in ClayFF force field development for molecular modeling of soil minerals and their interfaces with organic matter*
9:45 - 10:15	Eva Scholtzová *Clay minerals – useful adsorbents for drugs*
10:15 - 10:45	Ayesha Asbat *DFT-D3 evaluation of PMOx-modified smectite clays for toluene adsorption: towards sustainable VOC remediation*

10.45 – 11.15 Coffee break and posters

11.15 – 12.15 Soil minerals (Chair: Daniel Tunega)

11:15 - 11:45	Adyant Agrawal *Salt precipitation in porous media: atomistic coupling of hydration and electrostatics*
11:45 - 12:15	Katja Emmerich *Homoionic trans-vacant and cis-vacant montmorillonites: a density functional theory study*

12.15 – 13.15 Lunch and posters

13.15 – 15.00 Fate of contaminants in soils (Chair: Leonard Böhm)

13:15 - 14:00	James Kubicki *Molecular modeling of adsorbed species and kinetics*
14:00 - 14:30	Monica Shree Chandramohan *Spatial mapping and predictive modeling of potentially toxic elements in urban and peri-urban agricultural soils of Rome*
14:30 - 15:00	Jakub Ličko *How is actinyls' adsorption on clays affected by the presence of ligands? - A molecular dynamics study*

15.00 – 15.30 Coffee and posters

15.30 – 16.30 Fate of contaminants in soils (Chair: Chris Oostenbrink)

15:30 - 16:00	Saurabh Kumar *Environmental fate of antibiotics in Indian soil and complex water matrices*
16:00 - 16:30	Leonard Böhm *Elucidating clay mineral–organohalogen compound interactions: insights from laboratory experiments and molecular modeling*

16.40 – 17.20 VSOMM Demonstration

19.00 Heuriger – Conference dinner (Fuhrgassl-Huber – Neustift)

Friday, September 26th 2025

9.00 – 10.45 Soil organic matter (Chair: Chris Oostenbrink)

9:00 - 9:45	Mikhail Borisover *Complexity of soil organic matter: from chemical richness to metastability*
9:45 - 10:15	Dongqi Wang *Dynamics of humic acid and its interaction with uranyl*

10.15 – 10.45 Coffee and posters

10.45 – 11.45 Soil organic matter (Chair: Edgar Galicia-Andrés)

10:45 - 11:15	Hans Lischka *Pancake bonded radical PAH clusters as structural features in carbon nanomaterial*
11:15 - 11:45	Lorenz Dettman *Coarse-grained models for the investigation of the pollutant behavior in soil organic matter*

11.45 – 13.00 Interactions of minerals and SOM (Chair: Daniel Tunega)

11:45 - 12:30	Ashour Ahmed *From fundamentals to smart fertilizers: phosphorus simulations for sustainable soil solutions*
12:30 - 13:00	Ingrid Kögel-Knabner *Exploring microscale soil process complexes: insights from NanoSIMS*

13.00 – 14.00 Lunch and posters

14.00 – 15.30 Interactions of minerals and SOM (Chair: Daniel Tunega)

14:00 - 14:30	Franz Zehetner *Mineralogical changes and their impact on soil organic carbon sequestration and phosphorus availability along a one-million-year soil chronosequence*
14:30 - 15:00	Valentina Erastova *Let’s talk about dirt: from environmental sorptive materials of earth to biosignatures in space*
15:00 - 15:30	Kai Uwe Totsche *From atom to pedon: unravelling the structure-property-function nexus during weathering and pedogenesis*

15.30 – 16.00 Concluding discussion, remarks and farewell

3. Abstracts

Impact of computer simulations in soil science

Edgar Galicia Andrés

BOKU University, Institute of Molecular Modeling and Simulation (MMSI), Austria

Since the 1980s, computer simulations have increasingly shaped our understanding of soil processes at different scales and methodologic approaches, i.e., at the quantum mechanical level; molecular modeling and more recently the machine learning approaches. They are intended to reveal the dynamic behavior of soil components, such as to investigate mineral–organic interfaces, hydration, and sorption phenomena in complex soil systems.

One major step to model the organic fraction of soil is the development of the Vienna Soil Organic Matter Model (VSOMM), which contrary to first SOM models, it captures the chemical heterogeneity observed in natural systems. Moreover, our results exhibit the formation of mineral-associated organic matter (MAOM) which is correlated with the SOM organic composition.

These advances have provided with new applications in material science, promise new bioremediation solutions and even explanations behind the formation and stabilization mechanisms of soil organic matter (SOM), critical to provide a carbon sequestration solution.

Computational perspectives on soil interface phenomena: strength, ion transport, and PFAS retention

Hessam Yazdani

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Soil systems are complex and dynamic interfaces where mineral surfaces, water, and organic or anthropogenic constituents interact across spatial and temporal scales. Molecular dynamics (MD) simulations offer a powerful approach to interrogating these interactions at atomistic resolution, revealing mechanisms otherwise obscured in macroscale observations. This talk synthesizes MD-based insights from three distinct soil science and engineering investigations, each aimed at resolving interfacial processes critical to environmental and geotechnical performance.

The first study focuses on biocementation, a nature-inspired ground improvement technique that enhances strength and reduces permeability by precipitating calcium carbonate (CaCO3) in the pore space. While field-scale trials have demonstrated its promise as a sustainable alternative to traditional chemical grouting, the microscopic bonding mechanisms between CaCO3 and soil grains remain poorly understood. MD simulations show that CaCO3 adheres more strongly to quartz than to hematite or marcasite surfaces, especially under dry conditions. These insights reveal why biocementation is more effective in clean sands and suggest that mineralogy and saturation conditions critically influence treatment success.

The second study investigates chloride retention in stormwater infiltration systems amended with biochar. Nitrogen-rich biochars—modeled on algal feedstocks—demonstrate strong electrostatic and hydrogen bonding interactions with Cl^-, as shown by MD and density functional theory results. These findings support the design of functionalized biochars for dual-use in contaminant sequestration and carbon storage.

The third study addresses the transport of per- and polyfluoroalkyl substances (PFAS) in variably saturated aquifers. MD simulations confirm that PFAS adsorption is energetically unfavorable on quartz but favorable on carbonaceous biochar surfaces, explaining delayed breakthrough in amended systems.

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Claycode: a Python toolkit for modelling realistic clay systems

Hannah Pollak, Matteo T. Degiacomi

University of Edinburgh, United Kingdom

Clay minerals exhibit a wide range of properties and uses. They are employed as waste disposal barriers, pollution sequestration agents and pharmaceutical excipients, and their presence in the environment strongly influences soil properties, fertility, and the fate of contaminants.

Their physicochemical behaviour is closely linked to their molecular assembly, and slight perturbations in clay structure can significantly affect their performance. Molecular modelling techniques provide atomic-level insights that can guide experimental approaches and help unravel the mechanisms behind observed phenomena. However, models used in molecular dynamics simulations often rely on oversimplified clay structures, limiting the accuracy and representability of computational predictions.

We present ClayCode [1], a Python package developed to facilitate the modelling of clay systems that closely match their experimental counterparts. As an output, the user obtains a realistic clay model, parameterised with the ClayFF force field [2] along with input files for simulations using the GROMACS engine [3]. Besides the assembly of clay models from unit cells within an internal structure database, ClayCode also supports the creation of custom clay models from custom unit cell geometries supplied by the user.

Although still a relatively new tool, ClayCode is a promising addition to the molecular modelling toolkit and has already shown its value for building a range of realistic clay structures. The importance of using representative clay models in molecular modelling studies has been demonstrated in a benchmarking study on competitive barium and sodium adsorption, which is relevant to nuclear waste disposal.

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Characterization of solid/liquid interfaces by computational nonlinear optical spectroscopy

Milan Předota[1], Patrik Musil[1], Nijat Shukurov[1], Daniel Tunega[2], Moira Ridley[3], Arianna Marchioro[4]

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The ability to characterize surfaces is of paramount importance for many scientific fields. Heterogeneous catalysis, electrochemistry, lubrication, (bio)membrane functions and geochemistry, amongst others, all rely on the interaction of molecules at surfaces and interfaces. Nonlinear optics (NLO) methods such as second harmonic generation (SHG) and sum frequency generation (SFG) are in this regard well suited to probe surfaces and interfaces.

We will present a computational approach for processing of classical molecular dynamics (CMD) computer simulations of liquid at solid/liquid interface to determine the non-resonant second-order susceptibility $\chi(2)$ from the hyperpolarizability β of individual molecules parameterized by quantum calculations. We apply the method for microscopically flat surfaces, but the results can also be used to scattering from spherical particles (second harmonic scattering, SHS) in colloidal dispersions. We will demonstrate the effect of the surface charge density and salt concentration on the second-order nonlinear response of NaCl aqueous solution in contact with (101) quartz surfaces.

Resonant Vibrational Sum Frequency Generation (vSFG) is another excellent method for investigation of surfaces and interfaces, providing information on the orientation of bonds (O-H, C-H) at the interfaces and strength of their interactions, measurable by heterodyne by phase-resolved resonant SFG spectroscopy, where a pulsed polarized broadband IR (ωIR) laser beam is mixed with a tunable polarized VIS (ωVIS) beam to produce an output at the sum frequency (ωSFG=ωIR+ωVIS). We present computational predictions of the phase-resolved resonant SFG susceptibility $\chi(2)(\omega)$ of water at planar solid/liquid (quartz/water, alumina/water) aqueous solutions interfaces.

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The role of explicit polarizability in molecular modeling of clay-water interfaces across hydration states

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Clay minerals are key constituents of soils where their nanoconfinement properties control a wide range of environmental and technological processes, including contaminant retention, swelling, mineral weathering, and ionic transport. Because of the strong role of short-range electrostatic interactions, molecular dynamics (MD) simulations are a valuable approach to investigate how charged surfaces affect the structure and mobility of confined fluids. However, the predictive power of MD strongly depends on the choice of force fields. Developing reliable molecular-scale models is therefore critical to accurately describe clay systems under variable conditions. While non-polarizable force fields like ClayFF have been extensively used due to their computational efficiency and wide compatibility, incorporating explicit polarizability can provide a more realistic description of interfacial and nanoconfined fluid behavior.

This talk will present a comparative MD study of a montmorillonite mesopore at different water saturation levels, ranging from fully saturated conditions to systems containing only an adsorbed water layer on the clay surface. We performed MD simulations using the polarizable ion model (PIM) force field [1,2] and the widely used ClayFF reference force field [3]. Our results highlight marked differences in ion localization and water structuring between the two approaches. Under saturated conditions, PIM predicts enhanced ion pairing and long-range ordering in the diffuse layer, in contrast to the smoother profiles obtained with ClayFF and continuum Poisson–Boltzmann descriptions [4]. At low saturation, the deformation of surface cavities into more ditrigonal shapes observed in PIM simulations leads to a partial exclusion of cations from adsorption sites, resulting in a more homogeneous hydration of the clay surface. Conversely, ClayFF predicts partial surface dehydration driven by the localized trapping of cations near clusters of isomorphic substitutions.

Interestingly, despite these contrasting structural features, the averaged in-plane water diffusion coefficients remain similar across force fields. However, resolving diffusion components along orthogonal directions reveals a pronounced anisotropy in ClayFF under strong desaturation, attributable to heterogeneous wetting patterns. This directional dependencewas not observed with PIM, indicating a more isotropic interfacial dynamics [5]. These findings emphasize the significant impact of explicit polarizability on the predicted properties of clay–water systems, particularly under unsaturated conditions relevant to environmental and engineered scenarios such as deep geological repositories or soil remediation.

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Recent advances in ClayFF force field development for molecular modeling of soil minerals and their interfaces with organic matter

Andrey Kalinichev

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Molecular-level understanding of complex interactions between soil minerals, aqueous solutions, and dissolved organic matter is crucial for quantitative understanding and prediction of many processes in nature and in various technological applications, including mineral weathering, geological carbon sequestration, water desalination, geological disposal and storage of radioactive waste, etc. Modern methods of computational molecular modeling are capable of providing a greatly improved picture of the specific effects of the substrate structure and composition on the structure, dynamics and reactivity of the interfacial and nano-confined fluid phases.

However, accurate and realistic molecular scale simulations of soil minerals, such as clays, are often challenging because of the great diversity of their chemical composition, the significant degree of their structural and compositional disorder. ClayFF was originally developed in response to a strong need for a robust and flexible force field for classical atomistic simulations of such materials and interfaces, as well as their interactions with organic molecules in aqueous environment [1]. This talk will provide a brief overview of the fundamental assumptions and limitations of the ClayFF approach to the atomistic modeling of these complex systems, followed by select examples of the most recent ClayFF application to the simulations of a wide range of soil-related systems, focusing on the most recent improvements of the original ClayFF parameterization for better agreement with experimental data [2-5].

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Clay minerals – useful adsorbents for drugs

Eva Scholtzová

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Drugs, present in waste waters as pollutants, for example, excreted by human bodies, pose a big problem for the sustainability of the green environment. Suitable and effective adsorbents are necessary. Clay minerals are abundant, low-cost materials which can be used for environmental applications. They possess a large specific surface area, high porosity, surface charge, and diverse surface functional groups, enabling them to act as effective adsorbents and filters. Moreover, their surface properties can be chemically modified—from hydrophilic to hydrophobic—enhancing their suitability as adsorbents and carriers for organic compounds.

In the two presented studies, the models of drug-clay hybrid structures were used to study: 1. Stability of intercalated Rifampicin antibiotic drug to montmorillonite (RIF-Mt) and 2. Immobilising benzethonium chloride (antiseptic and anti-infective properties) by Mt (2:1 type) and kaolinite (Kaol, 1:1 type). The density functional theory (DFT) method with the D3 scheme for dispersion corrections implemented in the VASP program was used for examination. The findings are in good agreement with experimental results.

Acknowledgement: ES is funded by the EU Next Generation EU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V04-00009.

DFT-D3 evaluation of PMOx-modified smectite clays for toluene adsorption: Towards sustainable VOC remediation

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The functional modification of clay minerals with organic polymers has gained considerable attention due to its potential in developing high-performance materials for environmental applications [1]. Among the various approaches to pollutant removal, adsorption is recognized as one of the most effective and economically viable methods, particularly for capturing volatile organic compounds (VOCs) such as toluene, which is a hazardous aromatic hydrocarbon, and widely present in industrial effluents and poses significant environmental and health concerns [2].

In this study, we investigated the adsorption behavior of toluene on clay–polymer hybrid composites using Density Functional Theory with D3 scheme for corrections of disspersion forces (DFT-D3) [3]. Two smectites, e.g., saponite (Sap) and montmorillonite (Mt), were surface-modified with poly(2-methyl-2-oxazoline) (PMOx) to enhance their adsorption capacity and structural characteristics [4]. The hybrid systems, Sap+PMOx and Mt+PMOx, were examined for structural stability, interaction energies, and hydrogen bonding characteristics to understand their toluene adsorption potential.

Computational results indicated that the Sap+PMOx composite demonstrated a stronger adsorption affinity towards toluene than Mt+PMOx. However, they attributed to more favorable dispersion interactions and improved surface functionality. These findings suggested that PMOx-functionalized saponite is a promising candidate for VOC removal in water treatment and environmental cleanup technologies.This work provides valuable theoretical insights into the design of advanced clay–polymer adsorbents, contributing to the development of efficient, sustainable strategies for industrial pollutant remediation.

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Salt precipitation in porous media: atomistic coupling of hydration and electrostatics

Adyant Agrawal

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Soil salinization, due to evaporation-driven salt precipitation in porous media, is a pressing environmental challenge. Water transport through the porous media not only sustains crystal growth under confinement but also generates high crystallization pressures capable of damaging material's structure. Recent research suggests that interfacial phenomena, including water structuring, atomic roughness and surface charge critically influence water transport properties in porous salt crusts [1,2].

We use large-scale molecular dynamics, adsorption free-energy calculations, and NMR relaxometry to examine salt-specific precipitation mechanisms of three common salts—NaCl, KCl, and Na2SO4. We find that although the net crystal growth for all three salts proceeds linearly over microsecond timescales (with similar rates), their growth morphologies differ strikingly. Our analyses reveal that crystal morphology is governed by the interplay between ion-specific hydration and interfacial electrostatics. KCl exhibits smooth, layer-by-layer growth facilitated by balanced interfacial cation-anion adsorption. Whereas NaCl and Na2SO4 develop rough, water-retaining surfaces due to preferential Na+ adsorption, facilitated by the ion's strong-yet-frustrated hydration structure. In Na2SO4, strongly hydrated ions induce a dense, immobilized interfacial water layer that integrates into the lattice. Next, we identify anomalous crystal growth arising from specific defect topologies such as steps and kinks on NaCl surfaces. These defects significantly alter local adsorption energies, creating favorable sites selectively occupied by ions or water molecules. Finally, we relate these molecular-scale mechanisms to their influence on crystallization pressure under confinement, providing insight into the role of interfacial hydration and electrostatics in salt-induced soil degradation.

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Homoionic trans-vacant and cis-vacant montmorillonites: a density functional theory study

Katja Emmerich, I. Nugraha, Y.-Y. Liu, A. Asaad, P. Thissen

Karlsruhe Institute of Technology, Germany

Swellable clay minerals, known as smectites, are very important in soils and sedimentary rocks. They are also crucial for geotechnical applications and various industrial uses due to their abilities in cation exchange, hydration, and swelling.

Numerous experimental studies on the hydration of homoionic smectites can be found in literature. However, structural heterogeneity of natural dioctahedral smectites [1,2] is the source of uncertainties in the interpretation of experimental data. Hence, computational studies are especially useful to understand the influence of structural features on the hydration and swelling of smectites [3]. Thereby, many studies were performed for Na-saturated trans-vacant dioctahedral smectites.

The present study is a continuation of [4,5] and focuses on montmorillonites (sensu stricto). Layer charge was varied between 0.125 and 0.5. Three different octahedral structures (tv Mgcis, cv Mgcis and cv Mgtrans) and four different interlayer cations (Na+, Ca2+, Mg2+, K+) were considered. The electronic structure, atomic geometry, and total energy of montmorillonite models were calculated by Density Functional Theory (DFT) as implemented in the Vienna Ab Initio simulation package (VASP version 5.3.4) and dispersion correction (DFT-D3) was applied.

DFT calculations confirmed that cis-vacant (cv) octahedral sheets are preferred over trans-vacant (tv) octahedral sheets in montmorillonites independent of the position of the Mg2+ substitution in the cv structures. The basal space of the anhydrous homoionic montmorillonites correlated with the layer charge and the ionic radius of the interlayer cations although their position in the interlayer is different in dependence of size and charge. Variation in the basal space resulted in different specific densities of the montmorillonites, which needs to be considered for calculation of porosity and saturation.

Part of this work was funded by the German Federal Ministry BMUV (contract 02 E 12001A) and a BIB MORA-LPDP Scholarship, Republic of Indonesia.

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Molecular modeling of adsorbed species and kinetics

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For 35+ years, density functional theory (DFT) has been used to model adsorbed species on soil minerals. By comparing independently-calculated structures and vibrations to observed EXAFS and IR/Raman spectra, the identity of surface complexes can be ascertained. Furthermore, the adsorption enthalpies can be estimated to understand the relative strength of various sorbents (e.g., organic acids versus phosphate). Recently, the same techniques have been used to measure and model sorption kinetics.

This talk will focus on examples of nutrients (P), contaminants (As), and bacteria (extracellular polymeric substances). The need for including molecular-level information in larger scale models will be discussed.

Spatial mapping and predictive modeling of potentially toxic elements in urban and peri-urban agricultural soils of Rome

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Urban and peri-urban agricultural (UPA) soils are integral components of sustainable city ecosystems, but they are increasingly threatened by the accumulation of potentially toxic elements (PTEs) from industrial, vehicular, and historical urban activities. In this study, we evaluated 59 topsoil samples from various UPA zones around Rome using X-ray fluorescence (XRF) and inductively coupled plasma mass spectrometry (ICP-MS). We mapped the distribution of 19 elemental contaminants, including Pb, Cu, Zn, As, and Ni, using QGIS.

Multivariate statistical methods such as principal component analysis (PCA), hierarchical clustering, and k-means spatial clustering revealed distinct pollution profiles associated with geological features and anthropogenic sources. Predictive risk zones were identified, and contamination hotspots were highlighted for further monitoring.

This work demonstrates a data-driven framework to support land-use planning and contamination mitigation strategies in urban agricultural areas. Future work may assess the long-term dynamics of PTEs under different land-use scenarios.

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How is actinyls' adsorption on clays affected by the presence of ligands? - A molecular dynamics study

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Deep geological underground storage is a preferred method for long-term disposal of radioactive waste. Thus, the long-term safety of these facilities upon the anticipated degradation of waste canisters after thousands of years needs to be ensured. Thanks to their adsorptive properties, high surface area, swelling abilities and low permeability, clay materials are to act as a natural barrier in these conditions, preventing radionuclides from contaminating the surrounding environment.

Our radionuclides of interest are two actinides – uranium and neptunium. The effectiveness of the clay barrier at retaining these actinides, particularly in their actinyl forms (UO22+ and NpO2+) is of great interest, due to their long half-lives and radiotoxicities.

However, the presence of small organic acids and carbonate ions may reduce the clay barrier's effectiveness due to actinyl-ligand interactions that inhibit adsorption. We therefore use molecular computer simulations to gain an atomistic understanding of these adsorptive and complexation processes. Our results reveal key differences in behaviour between the two actinyls, both in terms of their adsorptive and complexation tendencies, likely entirely attributable to the differences in charge between the two ions. Broadly, uranyl exhibits a greater propensity for adsorption, as well as complexation, than neptunyl. Adsorption and complexation free energy calculations helped to quantify and explain these differences in behavior. This study thus provides qualitative and quantitative insight into the interactions between actinyls, organic ligands, and hydrated clay surfaces with real-world implications on radioactive waste storage conditions.

Environmental fate of antibiotics in Indian soil and complex water matrices

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Antibiotics play a vital role in combating bacterial infections and have been widely utilized in both human and veterinary medicine. It inhibits or kills harmful microorganisms and increasingly used worldwide for treating infections. Antibiotic pollution in freshwater systems, especially in densely populated regions, is an emerging environmental and public health issue demanding immediate attention. The antibiotics can transport through surface water and runoff, leakage and percolation in ground water and adsorption and desorption in soil. The presence of antibiotic residues can have long-term consequences, including their accumulation in food chain and the facilitation of drug-resistant bacterial growth and transmission to human being. Antibiotics can persist in soil for a prolonged period and affect the soil microbiome, particularly the bacterial diversity. This study explores how Indian soil primarily black, alluvial, and red interact with antibiotics under varying temperatures and complex water matrices (rainwater, river water, and distilled water). Results show that while higher temperatures generally enhance degradation, the pattern is inconsistent, suggesting complex interactions driven by soil characteristics, water chemistry, and antibiotic properties. The adsorption of antibiotics varies with soils; red soil shows very less adsorption with adsorption constant (q) less than 10 mg/g while black and alluvial shows higher adsorption with 22-25 mg/l varying with temperature and water matrices. The experimental data were best fitted by a second-order kinetic model, indicating that the rate of antibiotic degradation is dependent on the concentration of both the antibiotic and interacting components within the soil-water matrix.

Elucidating clay mineral-organohalogen compound interactions: insights from laboratory experiments and molecular modeling

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Hydrophobic organic compounds (HOCs), such as halogenated aromatic hydrocarbons, can be very persistent in the environment and lead to adverse effects on humans and other biota. For the assessment of their environmental fate and risk, sorption processes are highly relevant. Especially interactions between HOCs and organic matter are intensively studied, whereas data on interactions with clay minerals (CM) are still scarce, especially in case of organohalogen compounds (OHC). For the mechanistic elucidation of OHC–CM interactions, laboratory experiments have been combined with molecular modeling, both for various OHC–CM systems [1].

This talk presents results from OHC–CM interaction studies with five halogenated benzenes (hydrophobicity range of log K_{OW} 2.6–6.5) as HOC representatives as well as twelve pure phyllosilicate CMs and 20 smectite-rich bentonites (used as mineral phases in laboratory adsorption experiments). Molecular modeling of interactions was performed at the density functional theory (DFT) level for the same five halogenated benzenes and montmorillonite models of varying mineral structure with and without explicit solvation.

Our results show that OHCs can adsorb to clay minerals in relevant extent [2,3], with a strong mutual influence of OHC and CM properties on the extent of adsorption [3]. Expectedly, the hydrophobicity of the OHCs played a crucial role for the extent of adsorption, but can be outweighed by mineral properties. Results from molecular modeling did align well with laboratory results, but partly deviated based on the hydration state [2,4,5].

In particular, our results: (i) indicate a general influence of CM properties on OHC adsorption with a wide variation of solid-liquid adsorption coefficients that varied over orders of magnitude (log K_d 0.9–4.5); (ii) provide mechanistic understanding of the influence of CM characteristics such as layer charge, exchangeable cations, particle size, and pore size distribution on adsorption; and (iii) elucidate the hydration state being critical both for the extent of adsorption energies as well as the type of interaction processes.

Overall, the results suggest a strong influence of specific OHC–CM interactions on the environmental distribution behavior of HOCs with relevance for their fate, transport, and retention in the environment, e.g. for landfill sealing and long-term source/sink phenomena in soils and sediments.

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Complexity of soil organic matter: from chemical richness to metastability

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Chemical Diversity and Structural Ambiguity. Soil organic matter (SOM) comprises a chemically diverse set of substances, often operationally defined, resulting in extraordinary molecular richness. Even highly purified fractions yield thousands of molecular formulas—implying an even greater number of isomers and stereoisomers. As a result, the molecular structures of SOM components remain largely unresolved. Analytical approaches capable of probing both types of SOM atoms and groups and their connectivities in intact soils are critically needed. In addition to experimental techniques, a promising strategy involves the application of mathematical approaches such as nonnegative multivariate curve resolution (MCR). Recent applications of nonnegative MCR to IR spectra of soils and organic matter-containing materials show how spectral unmixing can reveal chemically distinct, a priori unknown components [1, 2]. Extending this approach through data fusion across multiple spectral domains may expose consistent spectral “faces” of soil/SOM components—potentially linked to real molecular entities or associations.

Modeling in the Absence of Structure. The limited structural resolution of SOM components presents a fundamental challenge for realistic molecular modeling (although the lack of precise structural knowledge may, in part, be "compensated" by weak SOM specificity in various interactions). The Vienna SOM Modeller (VSOMM) addresses this challenge by assembling molecular building blocks randomly selected from a library, constrained by ^{13}C NMR data, into plausible structures. This conceptual framework allows systematic testing of whether compositional or structural distinctions affect the behavior of simulated SOM systems. Recent molecular dynamics simulations using VSOMM-derived humic acid (HA) structures have suggested a stepwise rather than cooperative aggregation process, raising questions about the stability and molecular size of HA assemblies [3]. This experience has highlighted the possible areas for future development: expansion and classification of building block libraries, greater variation in assembly sizes, introduction of size distribution and branching patterns, flexibility in ionization behavior, and inclusion of multivalent cations (e.g., Fe^{3+}, Al^{3+}). The incorporation of additional compositional and spectral constraints could be envisioned to further reduce the degrees of freedom in creating realistic SOM molecular structures.

Beyond Equilibrium. SOM likely exists far from equilibrium with respect to molecular conformations, nanoscale organization, and mineral interactions. Supporting evidence includes sorption–desorption hysteresis, irreversible fractionation, and changes induced by wetting–drying cycles. Sorption–desorption profiles of well-defined chemicals may serve as experimental probes for detecting the formation and persistence of metastable states. The non-equilibrium behavior may influence SOM properties more profoundly than compositional variability and may need to be addressed in linking experiments and modeling.

Open Questions and Modeling Tasks. Among many important questions suited for exploration via molecular modeling: (1) Do water-soluble SOM fractions indeed form stable supramolecular assemblies, or do they follow simple multiple aggregation–disaggregation equilibria? (2) How do we reconcile the reported >100 nm sizes of dissolved organic matter? (3) Can modeling reproduce water-soluble SOM–pollutant interactions (e.g., with polycyclic aromatic hydrocarbons) and test often-claimed roles of sorbate planarity, SOM pool size, and electron donor–acceptor interactions? (4) Is SOM fractionation on mineral surfaces governed by equilibrium or history-dependent processes? (5) Strong and cooperative effects of SOM hydration on organic chemical sorption: Do they represent thermodynamics? (6) Can molecular modeling simulate sorption-desorption hysteresis under low site occupancy, and what is the role of metastable states in such systems? (7) Regarding soil sorption of phosphorus—central to productivity—can modeling clarify not only competition with SOM but also the observed SOM-induced enhancement of phosphorus sorption?

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Dynamics of humic acid and its interaction with uranyl

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The application of nuclear fission energy brings concerns on environment and health, and calls for extensive study on the migration of actinides possibly leaked in the environment. Humic acids (HA) are organic substances widely distributed in the environment, and their amphiphilic nature complicates the migration of actinides. In order to understand the role of HA, molecular dynamics simulations have been conducted to analyze the interaction between HA and uranyl in the presence of carbon nanotube (CNT) and graphene oxides (GO). The CNT and GO are possible intruders in the environment accompanying with the development of nanotechnology, and used to mimic hydrophobic and hydrophilic surfaces, respectively.

The simulations show that in aqueous phase, uranyl and HA can build close contact spontaneously, driven by electrostatic interaction. The binding of uranyl to HA favors a more compact conformation of HA. The presence of CNT unfolds HA via π-π interactions with the aromatic rings of HA, while did not influence the interaction between HA and uranyl significantly.

The presence of GO can compete against HA to adsorb uranyl ions, and the coordination structure and the binding sequences of HA, uranyl and GO had a significant influence on the folding behavior of HA. The energy decomposition analysis indicates that the driving force of the interaction between uranyl and HA or GO was mainly electrostatic interaction, while that between HA and GO was mainly van der Waals interactions. In addition, the addition of HA or HA could significantly reduce the diffusion coefficient of uranyl and GO, which hindered their migration.

The work also provides molecular level of evidence on the transformation of a hydrophobic surface into a hydrophilic one via noncovalent functionalization by HA, which in turn affects the migration of HA and the cations it binds to.

Pancake bonded radical PAH clusters as structural features in carbon nanomaterials

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Pancake bonding represents an interesting intermolecular bonding type involving radical and diradical polycyclic aromatic hydrocarbons (PAHs) in stacked arrangements. It includes covalent contributions leading to stronger interactions in comparison to conventional non-covalent π-π stacking. The structure of PAH radical clusters capable of pancake bonding and their interaction with a surrounding nonreactive PAH environment is important for the understanding of carbon nanomaterials. From the analysis of hydrocarbons in flames, radical and diradical PAHs have been found important in the formation of condensed phase carbonaceous nanoparticles. Recent atomic force microscopy (AFM) studies showed that aggregated asphaltene compounds included intermolecular π-π stacking and the occurrence of pancake bonding between radical and biradicaloid PAHs was hypothesized. Structural ensembles of pure clusters of seven prototypical open-shell PAHs (the radicals phenalenyl, olympicenyl and fluorenyl, the biradicals triangulene and heptazethrene, and the biradicaloids pentacene and nonacene) and mixed clusters including closed-shell pyrene were investigated. Low-spin and high-spin aggregates were considered. Ensembles of PAH clusters were created by means of metadyanamics (MTD) simulations using the Conformer-Rotamer Ensemble Sampling Tool (CREST) and the quantum chemical tight-binding GFN2-xTB method. Stacking motifs were found to include pancake bonding up to dimers and trimers and general PAH aggregation up to pentamers. Additionally, σ bond formation was found to be common in the low-spin state and reduced aggregation.

Coarse-grained models for the investigation of the pollutant behavior in soil organic matter

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Institute of Physics, Germany

The molecular modeling of soil organic matter (SOM) poses a challenge due to its structural and chemical complexity. Yet, molecular-level insights of SOM are of great value for unraveling its behavior and interactions. The Vienna Soil Organic Matter Modeler 2 (VSOMM2) enables the generation of condensed phase models of SOM, allowing the investigation of its structural and dynamic properties, as well as its interactions with a vast spectrum of chemical compounds. However, the atomistic resolution limits the exploration of these models on larger time and length scales, which are particularly relevant for studying adsorption processes and molecular mobility. To address this, we developed a coarse-grained version of VSOMM2 within the Martini force field framework to enhance the simulation performance of SOM models.

The model's accuracy was benchmarked against atomistic simulations and thermodynamic properties. Enabled by the introduction of an automated parametrization procedure, diverse SOM compositions at varying hydration levels were efficiently investigated. The coarse-grained models are further applied to study the mobility of pollutants in heterogeneous SOM matrices, revealing insights into their prevalent interactions and dynamic behavior. Additionally, we investigated the adsorption of SOM molecules onto a nanoplastic surface, bridging the simulations to experimentally accessible length scales. This research complements ongoing efforts in understanding the fate of pollutants in terrestrial ecosystems and provides a transferable framework for future studies on SOM and its environmental interactions.

From fundamentals to smart fertilizers: phosphorus simulations for sustainable soil solutions

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Advances in molecular simulation techniques, enabled by increasingly powerful software and hardware, are transforming our ability to understand complex chemical systems. These approaches provide deep insight into molecular geometries, thermodynamics, reaction kinetics, dynamics, and spectroscopy across pure phases, solutions, and heterogeneous interfaces. Despite this progress, environmental systems such as soil remain underexplored in computational chemistry, primarily due to their inherent heterogeneity and multiscale complexity.

In this talk, I will show how molecular simulations can address this gap by focusing on the biogeochemistry of phosphorus (P), a vital yet often inaccessible nutrient in soils. Using a multidisciplinary framework that integrates computational chemistry with experimental efforts, I will demonstrate how molecular simulations can unravel the mechanisms of P binding, mobility, and availability at the mineral–organic interface. These insights can inform the design of more efficient, sustainable fertilizers, ultimately enhancing soil fertility, protecting water quality, and supporting agricultural systems.

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Exploring microscale soil process complexes: insights from NanoSIMS

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Nano-scale Secondary Ion Mass Spectrometry (NanoSIMS) is a powerful analytical technique that combines high-resolution imaging with precise quantitative measurements of elemental and isotopic compositions. With a spatial resolution of approximately 100 nanometers, NanoSIMS enables researchers to visualize the distribution of isotopically labeled compounds within microscale hotspots, offering unique insights into the structural and chemical complexity of intact soil and plant systems. This technique bridges the gap between structural and chemical analysis by simultaneously providing spatially resolved information on elemental and isotopic distributions. Its ability to target specific microenvironments—such as iron (hydr)oxides, clay minerals, bacteria, plant residues, and roots—makes it particularly valuable for studying dynamic processes at critical interfaces, including the root-soil interface. NanoSIMS plays a crucial role in advancing our understanding of complex soil process interactions by directly imaging processes at the microscale and identifying the key biological and geochemical players involved. It supports and validates conceptual models across various disciplines, particularly in tracing intricate plant-soil-microbe interactions. This presentation will begin with an overview of the technical principles of NanoSIMS and essential sample preparation methods. The core of the talk will feature selected case studies that demonstrate the application of NanoSIMS in exploring soil and plant microenvironments. These examples will highlight how NanoSIMS contributes to unraveling soil process complexes and deepening our understanding of the dynamics within the soil system.

Mineralogical changes and their impact on soil organic carbon sequestration and phosphorus availability along a one-million-year soil chronosequence

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The Galápagos Archipelago, a chain of islands formed by hotspot volcanism on the Nazca tectonic plate, exhibits a pronounced gradient in rock age, increasing from west to east with distance from the volcanic hotspot. This study investigates secondary mineral (trans)formation, soil organic carbon (SOC) accumulation and phosphorus availability along a humid soil chronosequence spanning 1.5 to 1070 ka. We combine traditional bulk analyses, like X-ray diffraction and Mössbauer spectroscopy, with synchrotron-based 2-D mineralogical and geochemical microanalyses.

In the youngest, andic soils (≤4.3 ka), the clay fraction was dominated by allophane and ferrihydrite. During this early stage of soil formation, SOC accumulation was substantial (21.5 kg/m2) while P availability was relatively low. By 26 ka, illitic-vermiculitic phases became predominant, SOC stocks declined to approximately 15 kg/m2, while P availability peaked. In the older soils (≥166 ka), kaolinite, hematite and gibbsite were the dominant minerals, SOC stocks exhibited a second peak (25.5 kg/m2), and P availability declined to lowest levels.

Our findings highlight the critical role of both, short-range-order minerals and pedogenic oxides, which occur at different stages of soil development, in stabilizing organic matter and binding phosphorus. However, the precise mechanisms underlying these processes remain unclear and warrant further investigation. In this context, molecular modeling approaches may represent a promising avenue.

Let's talk about dirt: from environmental sorptive materials of earth to biosignatures in space

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The focus of this talk is on natural materials and their role in the chemical processes on Earth and other rocky planets. I will discuss the complexity of two noteworthy natural materials - black carbons and smectite clays - and our approach to the development of their molecular models. Our goal is to facilitate uptake of molecular simulations for the study of these materials and processes at their interface, enabling their targeted development for pollution remediation, soil enhancement and numerous industrial applications. Furthermore, I will show how molecular simulations can assist in constructing mineral-assisted origin of life hypotheses, and in guiding our search for biosignatures in Space. With this talk, I hope to stimulate further discussions towards exciting new ideas.

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From atom to pedon: unravelling the structure-property-function nexus during weathering and pedogenesis

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Soil's functions are intricately linked to its dynamic, three-dimensional, physical structure and its physicochemical properties. This structure is a consequence of the hierarchical system of porous aggregates, which provides an enormous variety of habitats and harbors a vast biological diversity. Combined with the chemical heterogeneity of organic, inorganic, and biotic components, a huge and interconnected biogeochemical interface emerges for the biogeochemical and biophysical interactions that regulate soil's functions (Totsche et al., 2010). Processes at these interfaces, operating across scales from the atomic to the pedon, are crucial for the immobilization, storage, and transformation of matter, energy, and information within soil (Totsche et al., 2018). Recent advancements in spectroscopic, spectro-microscopic, and tomographic techniques have significantly enhanced our ability to explore soil architecture and internal dynamics with unprecedented detail, from the smallest building blocks to intact soil cores (Amelung et al., 2024). The combined application of these cutting-edge techniques holds immense potential for fundamentally understanding the mechanistic basis of soil processes and the emergent functions that evolve during weathering and mature during pedogenesis. While advanced instrumental analytical techniques offer transformative opportunities to investigate the structure-property-function nexus, significant methodological hurdles, particularly in big-data and multi-scale analysis, must be overcome to realize their potential fully. Research should prioritize efforts to anneal data from diverse analytical platforms, including omics, to construct comprehensive, multidimensional models with explanatory capacity for the dynamic linkage of soil structure, properties, and functions, and bridge the gap between molecular-scale observations and pedon-scale functions (Totsche et al., 2024). Such understanding will be essential to functionally link soil architecture with fluid flow and transport, microbial activity, elemental cycling, and structural stability, to project the future of and maintain soils essential services, i.e., fertility, groundwater recharge and quality, biodiversity, soil carbon sequestration, element cycling, and biomass production, under the conditions of climate and land-use change.

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4. Posters

Adsorption of short-chain perfluoroalkyl acids on montmorillonite clay using the DFT-D3 method

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Per- and polyfluoroalkyl substances (PFASs) are synthetic compounds containing fluorinated carbon chains and are typically terminated with carboxylate or sulfonate functional groups [1]. They are valued for their chemical stability and surfactant properties and are widely used in domestic and industrial applications. However, their persistence, mobility, and potential toxicity have raised significant environmental and health concerns. Short-chain PFASs, often used as alternatives to regulated long-chain variants, are increasingly detected in water sources despite their lower bioaccumulation potential [2].

Conventional treatments such as activated carbon and ion exchange are often ineffective in removing short-chain PFASs. As a result, clay-based materials, particularly organically modified smectites, have gained attention due to their low cost, natural abundance, and tunable adsorption properties. Organically modified montmorillonite (Mt) exhibits a high surface area, cation exchange capacity, and structural tunability, making it a promising material for PFAS remediation. Such modifications help convert the naturally hydrophilic clay surface into a more hydrophobic and positively charged surface, suitable for adsorbing negatively charged, hydrophilic PFAS molecules [3].

This study investigates Mt as a promising adsorbent for the removal of short-chain perfluoroalkyl acid substances. Density Functional Theory (DFT) calculations, implemented using the Vienna Ab Initio Simulation Package (VASP) [4], are used to explore the interactions in the proposed systems. Structural optimizations are carried out using the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) functional.

A comparative analysis is conducted for Mt interacting with perfluorobutanoic acid (Mt–PFBA), perfluoropentanoic acid (Mt–PFPeA), and perfluorohexanoic acid (Mt–PFHxA). The results confirm the stability of the hybrid systems and reveal structural variations that are influenced by the PFAS chain length. These findings support the potential of clays as effective, sustainable adsorbents for removing short-chain PFASs from contaminated water.

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Computer prediction of second harmonic generation at interfaces: NaCl aqueous solution in contact with (101) quartz surfaces

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The ability to characterize surfaces is crucial across various scientific fields. Heterogeneous catalysis, electrochemistry, lubrication, (bio)membrane functions, and geochemistry, among others, all depend on molecular interactions at surfaces and interfaces. Nonlinear optical (NLO) methods, such as second harmonic generation (SHG), are particularly well suited for probing these interaction.

In this work, we present a computational approach for analyzing classical molecular dynamics (CMD) simulations of liquids at solid/liquid interfaces to determine the second-order susceptibility, χ(2)(ω), based on the hyperpolarizability, β, of individual molecules, parameterized using quantum calculations. In this study χ(2)(ω) derived from molecular trajectories of an aqueous NaCl solution in contact with (101) quartz surfaces, reveal the influence of surface charge density (ranging from 0 to -0.12 C/m^2) and salt concentration (from 0 to 0.8 M) on the second-order nonlinear response.

Furthermore, we decompose the total signal into contributions from layers at varying distances from the interface, enabling us to distinguish the surface-specific contribution from that of the diffuse layer. We will demonstrate how surface charge density and salt concentration affect the second-order nonlinear response of an aqueous NaCl solution in contact with a (101) quartz surface.

Prediction of heterodyne-detected VSFG spectra from classical molecular dynamics simulations

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Charged interfaces attract much scientific attention due to their omnipresence in a wide range of natural and industrial environments since the surface of any material is the principal pathway for its interaction with its surroundings. The specific orientation of water molecules in proximity to the air/water or solid/water interface induced by the interface significantly varies the properties of the environment in comparison with the homogenous (bulk) behavior. During the last decades, nonlinear optics experiments, namely Sum Frequency Generation (SFG), Second Harmonic Generation (SHG), and Second Harmonic Scattering (SHS), as representatives of the second-order nonlinear optical techniques became respected and powerful tools for exploring various topics ranging from fundamental questions of molecular dynamics at liquid interfaces to more applied problems of material surfaces. These techniques are highly suitable for studying processes at surfaces and interfaces since the signal arises solely from the non-centrosymmetric regions at the interface. They provide direct information about the average orientation of the water molecules at the interface; monitor ion adsorption at the surface with micromolar sensitivity; infer interfacial electrostatic potentials, or even monitor the time-resolved evolution of interfacial processes.

We present an MD trajectory processing software to predict vibrational SFG non-linear optics spectra from classical molecular dynamics simulations of solid-liquid and solid-air interfaces. The computational method requires as input ab initio calculated parameterizations of change of dipole moment and polarization tensor of a water molecule upon its vibration. However, classical molecular dynamics simulations of non-polarizable flexible water models are utilized to obtain the trajectories to be analyzed. This strongly reduces computation costs compared to ab initio calculations and opens the possibility of studying larger systems for long periods of time. The analysis allows a detailed investigation of the origin of the SFG spectra, including contributions from water molecules differing in distance from the interface. The role of various parameters affecting the calculation, as well as the inclusion of so far often neglected cross-correlation terms in the evaluation of the necessary time-correlation functions on various interfaces will be discussed.

Structure, dynamics and hydrogen bonding at corundum-water interfaces

Moira Ridley[1], Edgar Galicia-Andrés[2], Daniel Tunega[2]

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The interaction of water with mineral surface plays a crucial role in the mobility and bioavailability of nutrients and contaminants in soils. Surface processes including adsorption, dissolution, precipitation, and biomineralization are strongly influenced by the atomic structure within the interfacial domain. The structure of interfacial water, which may be quite distinct from bulk liquid water, arises from interactions between water molecules and surface functional groups of the various mineral phases. Clay minerals and metal (oxyhydr)oxide phases are the most reactive soil minerals. Aluminum, including corundum (α-Al2O3), and iron oxide phases are often the most common, so can play an important role in controlling aqueous ion concentrations.

In this work, we used first-principle molecular dynamics simulations (FPMD) to examine the structure and H-bonding networks at four corundum–water interfaces. The corundum surfaces studied were (001), (012), (113) and (110), with each surface having distinct surface functional groups and topographies. Our results reveal distinct differences in the H-bonding networks at the four surfaces. On the (001) and (012) surfaces there are ~3.1–3.2 H-bonds per water molecule, whereas there are only ~ 2.8 H-bonds per water molecule on the (113) and (110) surfaces. The H-bond profile from the surface into bulk water shows a maximum of H-bonds immediately adjacent to the (001) and (012) surfaces. In contrast, at the (113) and (110) surface the number of H-bonds is level. We consider the (001) and (012) surfaces hydrophilic, while the (113) and (110) surfaces have a more hydrophobic character.

Surface complexation modelling of charged organic chemicals to iron oxide combined with MO/DFT

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In two recent studies surface complexation models were developed to describe the adsorption of the organic chemicals Glyphosate, a widely used herbicide and Perfluor Octanoic Acid (PFOA), a common PFAS, on the surface of the iron oxide goethite. In the applied CD-MUSIC model, the charge of the adsorbing organic chemical species is divided over three planes at different distances from the surface. This charge distribution (CD), can be freely fitted from macroscopic adsorption data leaving many degrees of freedom. Here we used MO-DFT to calculate the geometry of the organic molecule bound to an iron dimer, as a proxy for the oxide surface from which the charge attribution to the surface (zero plane) was calculated. We also used MO/DFT to calculate the theoretical IR spectra of the possible adsorbed glyphosate species, which may have different protonation states and binding denticity, to compare with experimental IR data and reveal glyphosate speciation. This research highlights the advantages of combining complimentary techniques, both experimental and modelling, on a microscopic and macroscopic scale, to gain insights which cannot be eluded by either of the techniques separately.

5. Participant list

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6. Additional Information

CECAM website for this workshop:

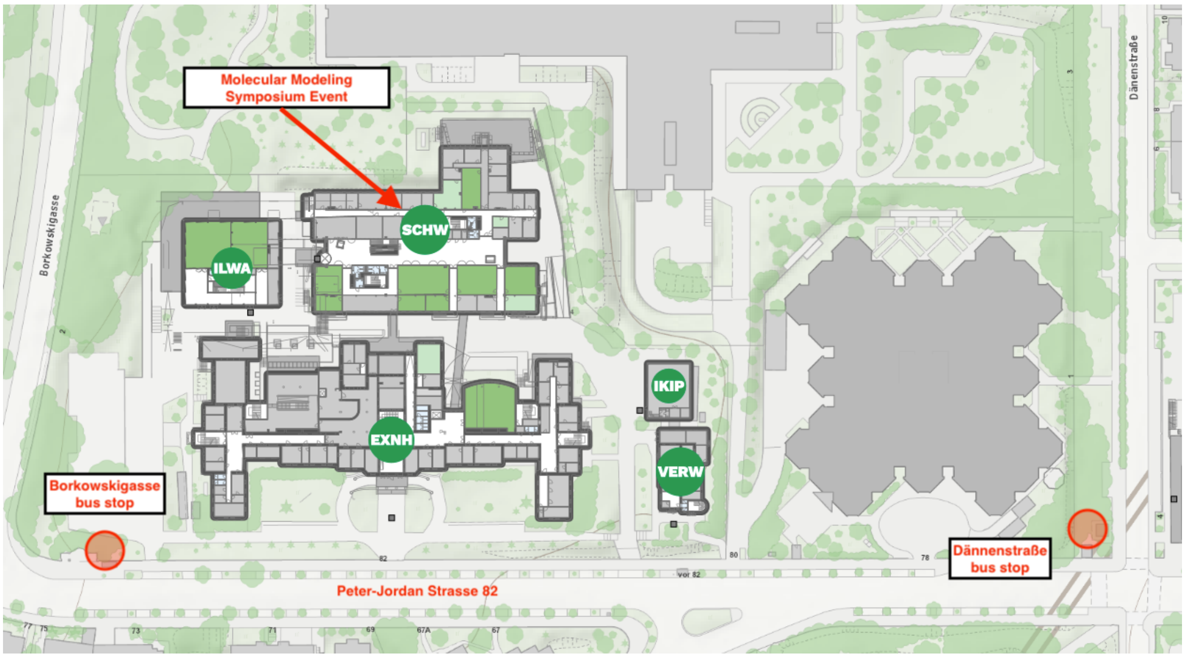
https://www.cecam.org/workshop-details/1393

Minerals Special Issue:

https://www.mdpi.com/journal/minerals/special_issues/G30922YKW8

Venue details:

Address: **BOKU University, Peter-Jordan-Strasse 82**, 1190 Vienna. **In Schwackhöferhaus "SCHW", Room 06**



Gala Dinner: Heuriger "Fuhrgassl-Huber" (Thursday 25th September 19:00)

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Notes: