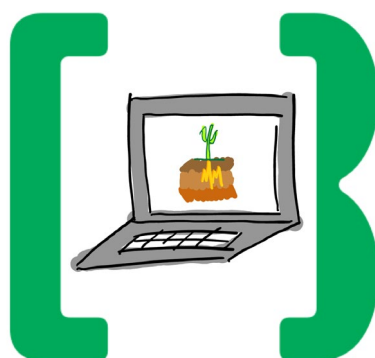


International Symposium 2025 Molecular modeling in soil science – achievements and perspectives



September 24, 2025 - September 26, 2025

CECAM-AT

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With the support of:



BOKU University



MDPI Minerals



Austrian Soil Science Society

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

[1] G. Sposito, *The Chemistry of Soils*, 2016

[2] K. Totsche, T. Rennert, M. Gerzabek, I. Kögel-Knabner, K. Smalla, M. Spiteller, H. Vogel, *Z. Pflanzenernähr. Bodenk.*, **173**, 88-99 (2010)

[3] J. Lehmann, M. Kleber, *Nature*, **528**, 60-68 (2015)

[4] A. Piccolo, *The supramolecular structure of humic substances: A novel understanding of humus chemistry and implications in soil science*, 2002

[5] A. Piccolo, R. Spaccini, D. Savy, M. Drosos, V. Cozzolino, *The Soil Humeome: Chemical Structure, Functions and Technological Perspectives*, 2019

[6] D. Šmejkalová, A. Piccolo, *Environ. Sci. Technol.*, **42**, 699-706 (2007)

[7] M. Gerzabek, A. Aquino, Y. Balboa, E. Galicia-Andrés, P. Grančič, C. Oostenbrink, D. Petrov, D. Tunega, *J. Plant Nutr. Soil Sci.*, **185**, 44-59 (2022)

[8] M. Gerzabek, D. Tunega, E. Galicia-Andrés, C. Oostenbrink, *Soil organic matter in molecular simulations*, 2023

[9] E. Galicia-Andrés, Y. Escalona, M. Gotsmy, C. Oostenbrink, D. Petrov, *Molecular Dynamics Simulations up to Earth: Modeling of Soil Organic Matter*, 2024

[10] R. Cygan, J. Greathouse, A. Kalinichev, *J. Phys. Chem. C*, **125**, 17573-17589 (2021)

[11] E. Iskrenova-Tchoukova, A. Kalinichev, R. Kirkpatrick, *Langmuir*, **26**, 15909-15919 (2010)

2. Program

Day 1 - Wednesday September 24th 2025

- 13:00 to 14:00 - Registration

Chris Oostenbrink, Daniel Tunega, Edgar Galicia-Andrés, Leonard Böhm, Martin Gerzabek

- 14:00 to 14:30 - Welcome & Introduction
- 14:00 to 14:30 - Christian Obinger (TBC)
- 14:00 to 14:30 - Sophie Zechmeister-Boltenstern (TBC)
- 14:00 to 14:30 - Andreas Baumgarten

Session: Advances of MM methods in soil science (Part I) 14:30 to 16:15

Martin Gerzabek

- 14:30 to 15:15 - Keynote: Edgar Galicia-Andrés
- 15:15 to 15:45 - Oral presentation
- 15:45 to 16:15 - Oral presentation
- 16:15 to 16:45 - Coffee break and poster session

Session: Advances of MM methods in soil science (Part II) 16:45 to 17:45

Chris Oostenbrink

- 16:45 to 17:15 - Oral presentation
- 17:15 to 17:45 - Oral presentation
- 17:45 to 18:15 - Poster Session

Day 2 - Thursday September 25th 2025

Session: Soil minerals (Part I) 09:00 to 10:45

Daniel Tunega

- 09:00 to 09:45 - Keynote: Andrey Kalinichev
- 09:45 to 10:15 - Oral presentation
- 10:15 to 10:45 - Oral presentation

Coffee break and posters session 10:45 to 11:15

Session: Soil minerals (Part II) 11:15 to 12:15

Martin Gerzabek

- 11:15 to 11:45 - Oral presentation
- 11:45 to 12:15 - Oral presentation

Lunch and posters session 12:15 to 13:15

Session: Soil organic matter (Part I) 13:15 to 15:30

Chris Oostenbrink

- 13:15 to 14:00 - Keynote: Mikhail Borisover
- 14:00 to 14:30 - Oral presentation
- 14:30 to 15:00 - Oral presentation
- 15:00 to 15:30 - Oral presentation
- 15:30 to 16:00 - Coffee break and poster session

Session: Soil organic matter (Part II) 16:00 to 17:00

Edgar Galicia-Andrés

- 16:00 to 16:30 - Oral presentation
- 16:30 to 17:00 - Oral presentation

Demonstration of VSOMM2 17:00 to 17:45

Edgar Galicia-Andrés

- 19:00 to 00:00 - Social dinner

Day 3 - Friday September 26th 2025

Session: Interactions of minerals and SOM (Part I) 09:00 to 10:15

Edgar Galicia-Andrés

- 09:00 to 09:45 - Keynote: Ashour Ahmed
- 09:45 to 10:15 - Oral presentation
- 10:15 to 10:45 - Coffee break and poster session

Session: Interactions of minerals and SOM (Part II) 10:45 to 12:15

Leonard Böhm

- 10:45 to 11:15 - Oral presentation
- 11:15 to 11:45 - Oral presentation
- 11:45 to 12:15 - Oral presentation
- 12:15 to 13:45 - Lunch and poster session

Session: Fate of contaminants in soils (Part I) 13:45 to 15:00

Leonard Böhm

- 13:45 to 14:15 - Keynote: James Kubicki
- 14:15 to 14:45 - Oral presentation
- 15:00 to 15:30 - Coffee break and poster session

Session: Fate of contaminants in soils (Part II) 15:30 to 17:00

Daniel Tunega

- 15:30 to 16:00 - Oral presentation: Leonard Böhm

- 16:00 to 16:30 - Oral presentation
- 16:30 to 17:00 - Oral presentation
- 17:00 to 00:00 - Closing Word

3. Participant list

Organizers

Böhm, Leonard

Justus Liebig University Giessen, Germany

Galicia Andrés, Edgar

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

Gerzabek, Martin

University of Natural Resources and Life Sciences Vienna, Austria

Oostenbrink, Chris

University of Natural Resources and Life Sciences, Vienna (BOKU), Austria

Slama, Karin

Institut für Bodenforschung, Austria

Tunega, Daniel

University of Natural Resources and Life Sciences, Austria

On-site participants

Ahmed, Ashour - University of Rostock, Germany

Borisover, Mikhail - Agricultural Research Organization - Volcani Institute, Israel

Kalinichev, Andrey - Institut Mines-Télécom Atlantique, France

Kubicki, James Kubicki - University of Texas at El Paso, United States

On-line participants

4. Additional Information

CECAM website for this workshop:

<https://www.cecama.org/workshop-details/1393>

Download the Planify app:

Notes:
