Aims & objectives

The objective of the thematic group Computational Chemistry and advanced physicochemical characterisation is the quantitative reconstruction and modelling of biogeochemical interfaces, their properties and interactions from the molecular scale to the higher BGI scales. BGl will be reconstructed on the basis of: original, artificial and model BGI’s, quantum chemical and molecular mechanics methods, using minimization techniques as well as Monte Carlo simulations and molecular dynamics simulations. Experimental approaches using advanced physicochemical characterisation methods.

The overall objective is to link the processes operative at the molecular scale to the phenomena active at the higher BGI scales in a mechanistic way.

Models of soil constituents and intermolecular interactions

- Lepidocrocite, goethite, montmorillonite, kaolinite, black carbon, carboxylic acid-based SOM models have been derived (Gerzabek et al., Totsche et al., Schaumann et al.)
- Sorption of PAH and Benthonite (Gerzabek et al., Totsche et al., Meleshyn)
- Calorimetric measurements and sorption isotherms (Kausch et al.)
- Atomic force microscopic (AFM) characterization of surface heterogeneity, morphology and topography of BGI’s. Force-distance and force-volume AFM measurements on column materials after reaction with phenanthrene (Totsche et al.)

Supramolecular associations

- Verification of experimentally predicted bridges of water molecules between SOM segments (Gerzabek et al., Schaumann et al.)
- Effects of hydration and cations in soil organic matter (Gerzabek et al., Schaumann et al.)
- Wettability of surfaces (Gerzabek et al., Bachmann et al.)

Discussion / conclusion

First steps in mechanistic understanding of physicochemical functioning of BGI’s are done or in work

- Sorption
- Hydration, cation effects
- Supramolecular structures
- Wettability

Challenges

- Further development of simulation techniques
- Transition to structured and heterogeneous surfaces and matrices
- Choice and improvement of modelling methods
- „Simplify“ and „complement“
- Design of experiments to verify models
- Models to verify hypotheses derived from experiments
- Advanced physicochemical characterization to achieve bridging of scales

References


Active group member projects and their contribution to TG 5

- Gerzabek (PI), Kaupenjohann (PI), Lang (PI), Siemens (PI), Krüger (Berlin): effects of hydration and cations in soil organic matter
- Schaumann (PI), Totsche, K. U., Rennert (Jena): Sorption of aromatic hydrocarbons to goethite.