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Towards understanding the interactions between hydrophobic organic compounds and clay minerals

PETER GRANCIC[1], LEONARD BÖHM[2], MARTIN GERZABEK[1] AND DANIEL TUNEGA[3]

[1]University of Natural Resources and Life Sciences
[2]Justus Liebig University Giessen
[3]University of Natural Resources and Life Sciences, Vienna, Department of Forest- and Soil Sciences

Presenting Author: peter.grancic@boku.ac.at

The sorption and desorption processes of hydrophobic organic compounds (HOCs) at reactive mineral surfaces pose a number of open questions. Since many of these compounds belong to the group of persistent organic pollutants, our understanding of their interactions with clay minerals and consequent bioavailability and accessibility is of vital importance in the risk assessment and management of soils and sediments. In this contribution, the interactions between HOCs (represented by hexachlorobenzene) and smectite clay minerals (represented by montmorillonite clay with varying number of isomorphic substitutions) are investigated via series of density functional theory calculations including both explicit and implicit solvent models. Based on the calculated electron densities, conclusions are drawn revealing the nature of their mutual interactions, the related stability of such complexes as well as possible molecular arrangements. A number of the calculated properties can be directly compared with experimental findings. These systematic studies aim to contribute to a better mechanistic understanding of the interactions of HOCs and reactive mineral soil surfaces. These calculations are complementary to a series of laboratory experiments, executed within the framework of our bilateral "ClayHOC" project.