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Schicksal, Wechselwirkungen und Wirkung von bodenfremden Stoffen im Boden

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Titel
Modelling of interactions of polar and nonpolar pollutants with soil minerals and soil organic matter

Abstract
Environmental pollution of soils by organic contaminants such as pesticides is one of the serious problems of our civilization. Contaminants can undergo various physical, chemical and biological transformation processes in soils governing behaviour, distribution, and fate of organic species in environment and subsequent environmental risks. Mechanistic understanding of molecular interactions of organic pollutants with main soil components represents a key factor for estimating the behaviour of contaminants in soils. Molecular modelling offers an opportunity to investigate and characterize various details of these interactions at molecular level providing specifications, which are difficult to obtain at the experimental level. This work represents a comprehensive overview of our investigations of the molecular interactions of organic contaminants with selected soil components. Particularly, we focused on the characterization of the structure and the surface complexation of the phenoxyacetic acid derivatives (herbicides MCPA and 2,4-D) and typical soil minerals such as clay minerals (kaolinite and montmorillonite) and iron oxyhydroxides (goethite and lepidocrocite). Further, interactions of several representative nonpolar polycyclic aromatic hydrocarbons (e.g. naphthalene, anthracene, pyrene, and phenanthrene) with iron oxyhydroxides were modelled, as well. It was found that in case of polar species, hydrogen bonds and electrostatic interactions play an important role in the formation of the surface complexes. In case of nonpolar PAHs, dispersion forces dominate in the planar stacking of the PAHs molecules on mineral surfaces. Another study focused at a complex 3D model representing humic substances firstly, featuring polar hydrophilic and nonpolar hydrophobic domains and also a nanopore SOM structure. This model was taken to simulate trapping and interactions of MCPA (polar) and naphthalene (nonpolar) species inside of the nanopore. It was found that MCPA is preferentially stabilized close to polar functional groups (carboxyl) whereas naphthalene interacts mostly with nonpolar aliphatic chains through dispersion interactions.