

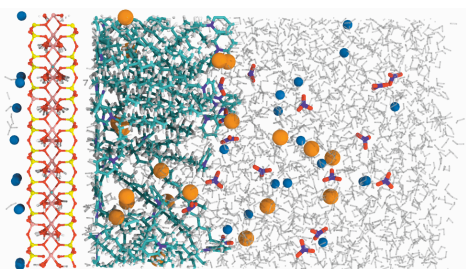
# Diffusion of ions in organically modified clays – experimental and molecular dynamics study

R. ŠOLC<sup>1</sup>, D. TUNEGA<sup>1\*</sup> AND B. SCHAMPERA<sup>2</sup>

<sup>1</sup>Institute of Soil Research, University of Natural Resources and Life Sciences, Peter-Jordan-Straße 82, A-1190 Vienna, Austria (roland.solc@boku.ac.at, \*correspondence: daniel.tunega@boku.ac.at)

<sup>2</sup>Institute of Soil Science, Leibniz University of Hannover, Herrenhäuser Straße 2, 30419 Hannover, Germany (schampera@ifbk.uni-hannover.de)

Organoclays exhibit for ions or non-polar compounds selective sorption ability, which depends on loading and structure of organic cations [1]. Organoclays based on montmorillonite modified by different amount of hexadecyltrimethylammonium (HDTMA<sup>+</sup>) and hexadecylpyridinium (HDPy<sup>+</sup>) cations were studied experimentally and by classical molecular dynamics (MD) simulations using the LAMMPS package (ClayFF, OPLS-AA, and SPC/E water force fields). The surface coating by organic cations was characterized by X-ray photoelectron spectroscopy (XPS) and atomic distribution profiles obtained from MD simulations. Diffusion coefficients (DCs) of the selected ions (Cl<sup>-</sup>, I<sup>-</sup>, NO<sub>3</sub><sup>-</sup>, SeO<sub>3</sub><sup>2-</sup>, and NH<sub>4</sub><sup>+</sup>) at the organoclay surfaces and in their nanopores were calculated from MD and compared with the experimental data.



**Figure 1:** Montmorillonite surface covered by HDPy<sup>+</sup> cations (bilayer arrangement) in a contact with NO<sub>3</sub><sup>-</sup> solution. (Blue balls - Na<sup>+</sup> cations, orange balls - Cl<sup>-</sup> anions, red-blue sticks - NO<sub>3</sub><sup>-</sup> anions).

The dependence of the calculated DCs on the different loading of the organic cations was observed from the MD simulations, in a correspondence with the experimental observations.

[1] Yariv (2002) *Organo-Clay Complexes and Interactions* 39-122, Marcel Dekker, New York, USA.