

Wetting of mineral surfaces – Molecular dynamics simulation

DANIEL TUNEGA^{1,2}, ROLAND ŠOLC¹, HASAN PAŠALIĆ²,
MARTIN H. GERZABEK¹ AND HANS LISCHKA²

¹Institute of Soil Research, University of Natural Resources
and Life Sciences, Vienna, Peter-Jordan-Strasse 82,
A-1190 Vienna, Austria

(*correspondence: daniel.tunega@boku.ac.at)
(rsolc@boku.ac.at, martin.gerzabek@boku.ac.at)

²Institute for Theoretical Chemistry, University of Vienna,
Währinger-Strasse 17, A-1090 Vienna, Austria
(hans.lischka@univie.ac.at, hasan.pasalic@univie.ac.at)

Wettability of minerals is primarily related to an energetic characteristic of surfaces affecting processes as adhesion, friction, detergency, biofilm growth, etc. The wetting ability of a solid surface is mainly determined by its chemical composition, structure and topography [1]. The solid-liquid contact angle method is often used to characterize wettability of surfaces and to determine its surface free energy.

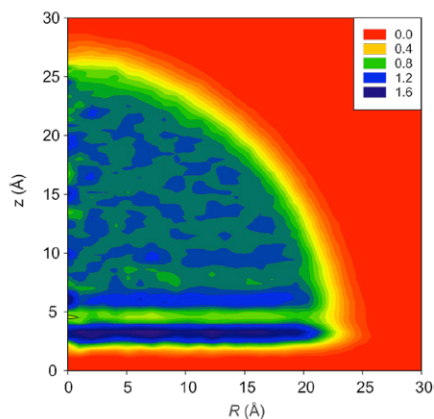


Figure 1: Visualization of water density profile (in g/cm³) of water droplet on the (001) tetrahedral kaolinite surface calculated for last 2 ns of MD simulation.

In order to elucidate structural and compositional factors affecting hydrophilic/hydrophobic character of minerals, interactions of water nanodroplets with basal surfaces of selected minerals (particularly kaolinite, goethite and lepidocrocite) were investigated by means of classical molecular dynamics simulations at room temperature. From the evolution and shape of the nanodroplet on the surfaces it was possible to characterize hydrophobic/hydrophilic character of studied surfaces.

[1] Bachmann, J. *et al.* (2000) *Soil Sci. Soc. Am. J.* **64**, 564–567.

Single particle ICP-MS for detection of engineered nanoparticles in environmental samples

JANI TUORINIEMI^{1*}, GEERT CORNELIS¹,
STEFAN GUSTAFSSON² AND MARTIN HASSELLÖV¹

¹Department of chemistry, University of Gothenburg,
Kemivägen 10 412 96 Gothenburg, Sweden

(jani.tuoriniemi@chem.gu.se, geert.cornelis@chem.gu.se,
martin.hasselov@chem.gu.se)

²Department of Applied Physics, Chalmers University of
Technology, 412 96 Gothenburg, Sweden
(stefan.gustafsson@chalmers.se)

Nanoparticles are used in increasing quantities in a vast number of products and concerns have been raised about possible harmful effects on health and environment. In order to study their fate and transport in different environmental compartments, methods that are sensitive, selective and capable of detecting extremely low concentrations of engineered nanoparticles among a high background concentration of natural nanoparticles need to be developed.

The established methods in trace metal analysis fail to distinguish between different types of particles, and other techniques (e.g. electron microscopy) can not provide quantitative information on a routine basis.

Single particle ICP-MS has showed promising potential for element-specific particle detection, by detecting particles as single intense spikes [1]. In this study, the technique is developed for complex environmental matrices and the capabilities and limitations of the technique for analysis and size estimation are explored.

Au and Ag standard nanoparticle suspensions have been used to show that an optimal dwell time exists between 1 and 10 ms for a specific nanoparticle size - background concentration combination where the spread in spike intensities is minimized, the sensitivity with respect to concentration is maximized while the (spike) signal-to-noise-ratio is kept high enough to detect the smallest particles in the sample. It was also possible to simultaneously measure the size and number concentrations of e.g. Ag nanoparticles, and the background concentration of dissolved silver, because nanoparticle spike intensities are independent from the dissolved signal.

Finally, application of the method to spiked natural waters and real treated waste water as well as road runoff is presented.

[1] C. Degueldre, P-Y Farvarger S. Wold (2006) *Analytica chimica acta* **555**, 263-268.