Goldschmidt 2026 Abstract
https://doi.org/10.46427/gold2026.36860

Physical adsorption of hydroxide ion at mineral-water interface

XIANDONG LIU

State Key Laboratory of Critical Earth Material Cycling and Mineral Deposits, Frontiers Science Center for Critical Earth Material Cycling, Nanjing University, Nanjing

Charging of mineral-water interfaces is a ubiquitous phenomenon in nature and lab. Interface charging plays a key role in various engineering and industrial fields. The most common mechanism for interface charging is the chemical adsorption of protons and hydroxide ions, such as the adsorption of protons on surface-exposed oxygen atoms and hydroxide ions on surface metal sites. Recently, with first-principles molecular dynamics (FPMD) simulations, we have discovered a novel interfacial charging phenomenon induced by physical adsorption of hydroxide ions. By taking corundum-(0001) as the model surface, MD simulations reveal that the negative charge originates from the physical adsorption of hydroxide ions from the solution, rather than from the deprotonation of surface hydroxyl groups or dissociation of interfacial water molecules. Detailed analysis indicates that the unique interfacial structure captures hydroxide ions from the solution through hydrogen bonding, thereby leading to negative interfacial charges. Extended simulations (FPMD, ReaxFF based reactive MD) show that hydroxide adsorption can also happen on other mineral interfaces, including (hydr)oxides and clay minerals. We have performed spectroscopy experiments to verify this novel charging mechanism. The effects of accumulated hydroxides on interface reactivity and precipitation will be discussed based on molecular modeling and experiments.

References

Zhang Y., Zhuang Y., Liu X., Cheng J., Lützenkirchen J and Lu X. 2024 Chemical Communications. DOI: 10.1039/D4CC01833H.

Zhang Y., Liu X., Gao P., Cheng J., Lützenkirchen J and Lu X. 2026 Geochimica et Cosmochimica Acta. DOI: 10.1016/j.gca.2026.02.008.