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Tracing Site-Specific Reactions at Mineral/Fluid Interfaces

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Mineral surfaces are reactive transformation centres and sinks for gases, solutes and solvents. Under environmental conditions these surfaces are populated by (hydr)oxo functional groups that can undergo protonation, ligand exchange, and form intricate networks of hydrogen bonds. Knowledge of the types, distributions and orientations of these groups is essential for understanding molecular-scale processes taking place at mineral surfaces.

This work is focused on the properties of hydroxo groups on important crystallographic planes of synthetic nano-sized iron and aluminum (oxyhydr)oxides exposed to vacuum, water vapor and/or carbon dioxide. Vibration spectroscopic signatures of hydroxo groups on these minerals will be presented alongside predictions from molecular dynamics simulations. This body of work forms the basis for a molecular-scale understanding of reactions taking place at surfaces of geochemically relevant mineral particles. These reactions are not only limited to ion and solvent exchange but are also extended to understand particle-particle interactions in the context of oriented aggregation.