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Computer Simulations at the Interface between Chemistry, Physics, and Soil Science: Advances in Understanding the Phosphorus Binding in Soil

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Molecular simulations have been developed to provide an indispensable tool in Chemistry and Physics as well as in related cross-disciplinary areas like Biochemistry, Biophysics, Chemical Physics, Materials science, and Astrophysics. Almost all areas of Chemistry are seen to benefit from the ever-increasing sophistication of numerical algorithms and computer hardware. Among the few topics that have not received much attention so far are biogeochemical processes occurring in soil. In this contribution, an interdisciplinary effort introducing multiscale atomistic simulation techniques into the field of soil chemistry will be presented. Here, the focus will be mainly on understanding the phosphorus (P) binding process in soil that is mainly affected by the strong interaction between P species and soil constituents and in particular mineral surfaces. The molecular-level reactions of P species (e.g., organic and inorganic phosphates as well as the most widely used herbicide "glyphosate") with mineral surfaces such as Fe- and Al-hydroxides have been studied using stationary calculations and molecular dynamics simulations based on different levels of theory involving quantum mechanics (**QM**), molecular mechanics (**MM**), and **QM**/**MM** hybrid approaches. Effects of different key factors (e.g., the chemical nature of P-compounds and soil constituents, crystal surface planes, binding motifs, water, solution pH, background electrolytes and their ionic strength, surface loading, redox potential, existence of free metal ions and organic matter) on the P binding process have been explored. Furthermore, we have developed and interpreted theoretical IR spectra that introduce a benchmark for characterizing experimental IR data for the adsorbed P species at Fe-containing minerals. In ongoing investigations, we are working on how to design new smart P fertilizers based on different bio-available materials such as phosphate-metal-humic complexes and bare and modified bone char (BC).

References

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