

Special Issue

Molecular and Chemical Studies of Organic Compound Behavior in Soils

Message from the Guest Editors

Soil science is an interdisciplinary science that is confronted today and for several decades with major societal, environmental, and human health issues. It has at its disposal a wide range of experimental and modeling techniques to address the issues at different scales of time and space. Its challenges concern, for example, the knowledge and control of pollution risks by contaminant molecules such as pesticides, drugs, pharmaceuticals, etc. The soil is a compartment of the ecosystem that significantly contributes to the global cycle of pollutants. In most cases, it serves as the major sink capacity and transformation reactor. The rapid progress in computer technology and in the development of computational methods in theoretical chemistry has allowed us to access to analyze complex systems such as soil and solvated contaminant systems and their interactions within biogeochemical interfaces. In this Special Issue, we welcome contributions from all fields of computational and theoretical chemistry, including reviews and original works, demonstrating the key role of soil, as an ecosystem compartment, in the global pollutant cycle.

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