Interaction energies in soil systems – molecular scale view

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Main natural soil components are represented by soil organic matter (SOM) and soil minerals (e.g., clays, iron oxyhydroxides, etc.). The composition and the structure of soil components are responsible for the formation of soil organo-mineral aggregates (SOMA), and consequently, for the stability of SOMA and their interactions and reactivity with environment. For example, adsorption and accumulation of environmental pollutants by soil components and SOMAs is one of the key functions of soils. Therefore, it is of outmost importance mechanistic understanding of processes responsible for the formation of SOMA and interactions of SOMA and soil components with various chemicals (e.g., organic pollutants such as pesticides) at the molecular scale.

In this presentation, several examples are shown how molecular modeling can contribute to exploring interactions of SOMA and soil components. Particularly, it demonstrated how kaolinite-humic acid (K-HA) microaggregates are formed and what is their stability with respect to chemical environment. Further, the origin of the interactions of organic pollutants such as glyphosate and chlorinated hydrocarbons with clay minerals is revealed. In these examples, the methods of molecular modeling such as classical molecular dynamics and/or density functional theory-based approaches are used.