ADSORPTION OF TWO PESTICIDES ON A CLAY SURFACE: A THEORETICAL STUDY

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The contamination of water resources with many organic xenobiotic compounds poses a challenge to environmental sciences and technologies [1]. Although in many cases these contaminants are present only in small concentrations, the large variety of such compounds (some of which are classified as priority pollutants) is a matter of concern. Adsorption, alone or as part of a more complex water or wastewater treatment process, has been seen as playing a very important role in the removal of many of these pollutants [2]. In this regard, the choice of adsorbent materials is crucial, which requires an understanding of the details involved in the adsorption of more or less complex organic molecules by a variety of surfaces of different types. In addition to laboratory studies, computational studies may be valuable in this study [3].

MCPA (2-methyl-4-chlorophenoxyacetic acid, a herbicide) and Clofibric acid (2-(4-chlorophenoxy)-2-methylpropanoic, the metabolite of a pharmaceutical, clofibrate, and also a herbicide) are two phenoxy acids that differ only slightly in their structures. However, a quite distinct behavior in adsorption phenomena on clay materials has been observed in past studies [4]. By relating those differences with the molecules' structural features through atomistic computational studies, some insight may be gained into the respective adsorption processes of this type of compounds.

In the present work quantum chemical calculations at density functional theory level have been performed to study the adsorption of MCPA and Clofibric acid by a clay surface model. Since hydration plays an important role for the adsorption process of these species, solvent effects were considered by inclusion of water molecules explicitly into the quantum chemical calculations.

The deprotonated negatively charged species were found to strongly interact with the surface and the distinct behavior of both species upon adsorption was compared with experimental evidences.

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