Adsorption of Contaminants on Clay Mineral Surfaces

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The accumulation and persistence of hazardous compounds (HCs) in surface and ground water as well as living organisms have emerged as an adverse effect of human anthropogenic behaviour. A variety of HCs, from emerging contaminants found in pharmaceutical residues and personal care products to household chemicals, biocides/pesticides and manufacturing wastes persist in the environment [1]. Some of these compounds have been shown to cause adverse effects in aquatic organisms as well as promote an increased risk of humans developing thyroid disorders, tumours and diabetes.

In this study, we aim to build on the foundations of our understanding of how HCs interact with the environment by applying atomistic simulation methods to determine the physicochemical factors controlling the distribution of pollutants and their metabolites in aqueous and terrestrial environments, and then apply this to identifying sustainable ways of control their transport. Additionally, it has been suggested that clay minerals could act as geosorbants for the remediation of organic pollutants [2], so an evaluation of their adsorptive properties would be useful.

In initial studies, HCs adsorption on two model clay surfaces, sodium montmorillonite and pyrophyllite were performed to calculate their binding free energy and identify favourable sites for adsorption, in vacuum and water, using dispersion corrected DFT and classical MD methods. Our initial investigation focused on 10 molecules including dibenzo-dioxins and two poly-chlorinated derivatives, chloro- and hexachloro-benzene, emerging contaminants amphetamine with two other derivatives and MDA and its analogue MDMA. These compounds were chosen to identify the links between the chemical properties of these HCs and their possible fate and effects in the environment.

[1] Margot *et al.* (2015) *WIREs Water* **2**, 457–487.
[2] Churchman *et al.* (2006) *Developments in Clay Science* **1**, 625-675.