

Figure 1: Pyrophyllite

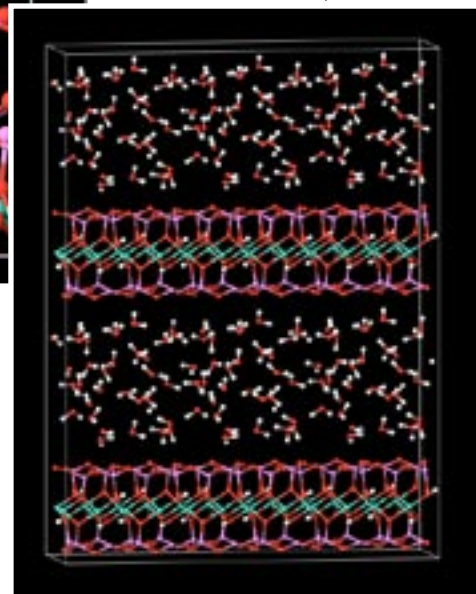


Figure 2: Pyrophyllite at the mineral/water interface.

e-Minerals: environment from the molecular level

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We are interested in the processes by which organic pollutant molecules (such as DDT, PCBD and dioxins) bind to soil minerals. This is important because of the wide range of industrial organic pollutants (e.g. DDTs, PCBs, dioxins) found in soils and increasingly being detected in the human food chain, together with the known problems for health and reproduction. An atomistic approach must account for realistic mineral surfaces in contact with fluids containing ionic components with variable pH, and the role of natural organic matter at mineral surfaces.

Initially we are focusing on the interaction 2,3,7,8-tetrachloro dibenzodioxin (TCDD) with the (001) surface of the layered clay mineral Pyrophyllite as a representative system. 2,3,7,8-TCDD makes an excellent test case because it is a known carcinogen and widely regarded as the most toxic of all the dioxin congeners and has been the focus of most experimental research into dioxins.

In total there are 419 dioxin (or dioxin-like) compounds. We intend to perform a systematic study of the interaction of all of

these compounds with a range of clay minerals. We estimate that this will take something in the region of 40,000 calculations for a single mineral surface (depending on the methodology). For a given mineral there may be a large number of relevant surfaces, moreover there are potentially thousands of minerals that one might wish to investigate. This is why we are investing so much in setting up these calculations. Certain calculations will need to be performed on extremely large systems and this is why having an optimised SIESTA running on HPCx is so important (and unlike some HPC facilities HPCx is Grid-enabled). Eventually, we want to look at more realistic systems, such as the 'wet' system shown in Figure 2.

This work is being conducted as part of one of the UK e-Science programs (e-Minerals: Environment from the Molecular Level). We are building an infrastructure for performing simulations that exploit the emerging Grid technologies using Globus and Condor. Our HPC focus is on performing simulations on environmentally relevant systems.