Computer modelling of the interface between alcohols and the (10.4) calcite surface

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Crystals grown in organic or biological environments often show more complex morphologies than those generated using more conventional methods. For this reason techniques allowing control of the size and shape of crystal growth in organic solutions are of current industrial and academic importance [1]. However, there still remains uncertainty over the exact mechanisms by which these processes progress. Computer modelling provides one route to improving our understanding of these processes [2, 3].

In this work we report initial results modelling the interaction between alcohol solutions and the (10.4) surface of calcite, which dominates the morphology of conventionally grown crystals, expanding on previous studies undertaken in this area. The DL_POLY 2 [4] molecular dynamics package has been used to simulate several alcohol-calcite systems. These simulations, and subsequent analysis, suggest that an increase in the carbon chain length of the alcohol results in a decrease of the interfacial energy, which infers that the longer chain alcohols are therefore less tightly bound to the calcite surface.

Analysis of the radial distribution functions (RDF), demonstrates that the distance between the surface Ca ions and the alochol oxygen in the adsorption layer is approximately 1.5 Å and the separation between the CO_3 oxygen and the –OH hydrogen to be around 2.5 Å, demonstrating that the strong interations exist between the molecules and the surface. This is further demonstrated when the density profile perpendicular to the surface is considered, where a highly ordered adsorption layer is observed together with less well defined secondary layers further from the surface.

Future work will extend this study to consider the interface between stepped calcite surfaces and alcohol and will also consider the co-adsoption of water and alcohol at the surface.

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Investigating organic–clay interactions

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The interaction between organic matter and layered minerals has played a role in shaping the past and the present of human life on Earth, and will continue to in future. We describe a range of computational and experimental studies to understand layered mineral - organic interactions.

In the Archean oceans, small molecules would have spewed out of hydrothermal vent systems, however without means of concentrating the organic molecules, the resulting dilute solution would not have allowed reactions to occur. We have used simulations to illustrate how clay minerals are able to both concentrate and react organic molecules and protect larger molecules [1, 2].

In modern times oil exploration has become ever cleaner, however legislation has also tightened. When drilling for oil, a technical fluid is used, which has to fill several roles including stabilizing clay shales against swelling. Water-soluble oligomer inhibitors are used to control swelling; a fundamental understanding of the clay-swelling inhibitor interaction is needed. We use computer simulations, and experiments, to understand the subtle interplay between different functional groups, clay types and hydration state [3].

We have made use of computational grids to run simulations at an unprecedented scale –millions of atoms – of clay polymer composites. These have shown the emergence of thermal undulations, enabling the calculation of materials properties of both the whole system, and the clay platelets [4].

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