Atomistic modelling of oxide and mineral interfaces

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The aim of this presentation is to describe recent work using atomistic simulation methods to model the structure, stability and reactivity of mineral surfaces. Initially, the ways in which the surface structures are generated and modelled using atomistic simulation will be reviewed. We will then describe several approaches for increasing the scope and reliability of the simulations, either by including the dynamical contribution to the surface stability, or by increasing the reliability of the description of the interactions, using electronic structure simulations. The application of these approaches to several materials will be discussed, including Al_2O_3, Fe_2O_3, MnO_2 and $CaCO_3$, which examine how the stability of the interfaces are modified by the presence of impurities and water. The results demonstrate that atomistic simulation techniques can provide a useful complementary tool for modelling oxide and mineral interfaces.