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Editorial

EDITORIAL NOTE ON MOLECULAR MODELLING

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EDITORIAL

Molecular modelling (MM) is another technique that provides atomistic insight into the mechanism of ion–mineral surface interactions. The most widely used simulation techniques are molecular dynamics (MD), Monte-Carlo, and geometry optimization. The equilibrium structures of sorbed species, as well as their energies, are calculated using inter-atomic interaction energy estimates based on statistical mechanics rules. The interatomic energies are determined either directly using quantum mechanics methods or indirectly using empirical interaction parameters calibrated using quantum-mechanical calculations or experimental data for simplified model systems. The system size and time scale that can be addressed in the modelling are the primary limits of MM simulations. Because of the tiny system size, the simulation can only handle relatively high solute concentrations. The simulations' computing expenses are frequently a trade-off between accuracy and efficiency. With the development of massively parallel computers, it is now possible to do a full quantum-mechanical computation based on density functional theory for systems with hundreds to thousands of atoms.

The choice of interaction potentials is especially important in simulations using empirical force fields. Because of the delicate balance between ion–solvent, solvent–solvent, and ion–ion interactions, accurately describing complicated solutions and interfaces is exceedingly difficult. Despite these drawbacks, MM simulations help us better understand how sorption processes work. The process of cation exchange in the interlayer, the surface complexation on the basal plane of different metal ions, and the influence of surface charge and hydroxylation on the sorption of different metal ions on the (110) surface of rutile have all been explained using classical MD simulations. To describe the structure of edge sites on clay minerals, estimate the acidity of the surface sites, and explain the process of ion surface complexation on the basal surface of clays, quantum mechanical simulations were used. A density functional theory technique was recently used to investigate uranium complexation of the edge of kaolinite.

In certain cases, idealised and oversimplified systems, atomistic simulations provide a 3D resolved explanation of sorption processes on mineral surfaces. Atomistic simulations, when combined with properly chosen spectroscopic and macroscopic tests, may be used to explore the structure and reactivity of mineral surfaces, as well as to establish limits on the number of potential surface sites by offering the energetically most favourable one.

Molecular modelling is a modern, cost-effective approach for creating novel molecules and chemical entities. Computer reports in the form of solely theoretical research or as complements to experimental work are becoming increasingly popular as computational resources become more available and more user-friendly molecular modelling software are developed. For example, Density Functional Theory (DFT) methods are now widely used for determining the electronic structure of organic molecules for the fabrication of electron or hole transport materials, in comparison to electrochemical methods such as Differential Pulse Voltammetry (DPV) measurements and in the development of photoinitiators.

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