review of Molecular Modeling of Clays and Mineral Surfaces (cms workshop lectures, Volume 12), edited by J.D. Kubicki and W.F. Bleam (The Clays Minerals Society, Aurora, CO) 2003, to be submitted to Powder Diffraction

by Eric Cockayne

Many issues in environmental science require understanding the interaction between soils, water, and sediments. For example, the containment of radioactive or chemical wastes is related to the ability of the constituent soil materials to chemically bind these materials. As available computational power has grown in recent years, molecular modeling has become an important tool in the field. This book gives an overview of state-of-the art methods and results in using molecular modeling to investigate the interaction of clay and mineral surfaces with water and with water containing solvents.

Chapter 1 gives an overview of molecular modeling methods. Different methods are preferred for different length scales. For systems containing tens of atoms, fully quantum mechanical solution of the electronic structure problem is preferred. For larger systems (generally including systems large enough to model the interaction of water and solutes with surfaces), empirical “force field” methods are preferred. The advantages and disadvantages of each method are discussed, as well as how hardware considerations affect the size of the system that can be practically simulated. The description of various packages available for molecular simulations will be useful to those wishing to incorporate molecular modeling into their research.

The subsequent chapters are devoted to the use of molecular modeling to investigate specific problems involving mineral surfaces and sorption. Chapter 2 discusses electronic structure methods for treating the interfaces between mineral surfaces and water. In chapters 3 and 4, force-field models are used to study the interaction of water and aqueous ions with clay surfaces. Chapter 5 presents a more abstract model, designed for the larger-length scale problem of how metal ions bind with chemically heterogeneous soil materials. These chapters discuss the power of molecular modeling to predict structure, thermodynamics, preferred binding sites, the dynamics of ion diffusion and binding, and the effects of pH on sorption.

Several common themes run through this volume. The importance of first understanding existing experimental results before making predictions is emphasized. Furthermore, modeling should not be done independently of, or thought of a replacement for experiments, but, in fact, even more experiments are necessary, not only to confirm the

modeling predictions, but also to provide necessary inputs for better models. Technical difficulties involved in modeling surfaces realistically are discussed. Finally, it is pointed out that it is still computationally expensive to get good agreement with experiments in many cases.

The faults of this book are some minor errors, oversimplification in the discussion of statistical mechanics and electronic structure methods in places, and the use of jargon and symbols that are not familiar except to specialists. Still, it provides a good overview for those who may wish to become more familiar with modeling the interactions of aqueous solutions with mineral surfaces, and leaves one with the hope that a combination of experimental and modeling methods will provide new solutions to related environmental and industrial problems.