Two remarkable properties that can be found on many mineral particles (clays, gibbsite, CSH, ...) are: their shape anisotropy due to their plate-like nature, and their ability to possess a charge anisotropy. The latest consists in basal faces bearing a negative structural charge whereas the rims present treatable sites which carry a positive charge at neutral-acid pH values and a negative charge in alkaline solutions. Both anisotropies are responsible for the complex behavior of plate-like particles in solutions. In this contribution, theoretical studies, using Monte Carlo simulations, of the properties of such particles in aqueous solutions will be presented.

In a first part, the acid-base behavior of 2:1 clays is investigated. We show that with a fairly simple model one can capture the charge formation of the clay particles in presence of a monovalent electrolyte. The results of this study also allow us to explain many phenomena that are experimentally observed [1].

In a second part, a theoretical investigation of a model clay dispersion in 1-1 salt solutions varying the particle volume fraction, ionic strength as well as the charge distribution on the clay platelets is presented. Simulations show a complex phase behavior, and all phases found experimentally are also found in the simulations. Repulsive and attractive liquid phases, as well as gel, glass and liquid crystal phases are reported. Nevertheless, we predict the formation of new liquid crystal phases that have not yet been experimentally discovered (Smectic B and exotic columnar phases) [2,3]. The influence of the previously cited parameters on the formation and stability of these phases will be discussed in light of experimental observations on clay suspensions.