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The role of Stern layer ions in ionic transport in porous media

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Understanding the role of Stern layer ions is crucial for assessing the ionic transport in nanochannels at high ionic strengths. Currently, MD simulations are one of the most promising tools to offer a realistic picture of the ionic behaviour close to charged surfaces where the Stern layer is located [1,2]. Experiments (like streaming potential and titration), on the other hand, are modelled using mean-field theories, like the Poisson-Boltzmann [3-6]. In this work, we show how the results of experimental investigations, interpreted using mean-field theories can be used to validate the results of MD simulations.
Specifically, a charged amorphous silica surface in contact with an electrolyte will be considered. The Stern layer is defined as the layer that starts at the surface of the silica and extends to a position where Poisson-Boltzmann starts to be valid. In the Stern layer, which has a thickness of a few Å, it is impossible to assume that ions are point-like, as this leads, especially at high ionic strengths, to unrealistic ionic densities. To account for a Stern layer, it is customary, in mean-field models, to model this region of space as a capacitor. The difference between the electric potential at the silica surface and the electric potential at the end of the Stern layer is then said to be equal to the surface charge density divided by the Stern layer capacitance (in F/m^2). The value of this capacitance can be estimated by modelling either by titration or by streaming potential measurements, for this capacitance is the only adjustable parameter in the model. We will show, in a first step, how the value of this Stern layer capacitance influences the ionic transport in streaming potential measurements and affects titration results. In a second step, we will compare the value found for the Stern layer capacitance with the results obtained from MD simulations. As the Stern layer capacitance is a function of both the Stern layer thickness and its permittivity, we will be able to discuss the value of the relative permittivity in the Stern layer.

Participation

In-Person

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