Abstract Submitted
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**Coarse-graining, Electrostatics and pH effects in phospholipid systems**[1] ALEX TRAVESSET, Iowa State University and Ames Lab, SWETA VANGAVETI, Iowa State University — We introduce a minimal free energy describing the interaction of charged groups and counterions including both classical electrostatic and specific interactions. The predictions of the model are compared against the standard model for describing ions next to charged interfaces, consisting of Poisson-Boltzmann theory with additional constants describing ion binding, which are specific to the counterion and the interfacial charge ("chemical binding"). It is shown that the "chemical" model can be appropriately described by an underlying "physical" model over several decades in concentration, but the extracted binding constants are not uniquely defined, as they differ depending on the particular observable quantity being studied. It is also shown that electrostatic correlations for divalent (or higher valence) ions enhance the surface charge by increasing deprotonation, an effect not properly accounted within chemical models. The model is applied to the charged phospholipids phosphatidylserine, Phosphatidc acid and Phosphoinositides and implications for different biological processes are discussed.

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