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Enhancing and reversing the electric field at liquid/liquid interfaces YUFEI JING, GUILLERMO GUERRERO GARCIA, MONICA OLVERA DE LA CRUZ, Department of Materials Science, Northwestern University, Evanston, IL 60208, USA — The ion distribution at the interface between two immiscible electrolyte solutions determines the macroscopic properties of these liquid interfaces. The classical Poisson-Boltzmann theory has been widely used to describe it, even though it neglects the polarization and ion correlations typical of these ionic solutions. Here, we provide an enhanced description of a liquid/liquid interface in the presence of an electric field from first principles—that is, without needing any fitting parameter—including ion correlations, image charges and realistic ion-sizes in Monte Carlo simulations. Our data agree well with experimental excess surface tension measurements for a wide range of electrolyte concentrations, contrasting with the results of the classical Poisson-Boltzmann theory. More importantly, we observe that, in the vicinity of the point of zero charge, the electric field can increase significantly in strength near the liquid interface, or it can even reverse locally, at high salt concentration.

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