

GOAL: Analyze the effect of multivalent electrolyte solutions on charged interfaces, electric double layers, though the application of computational methods

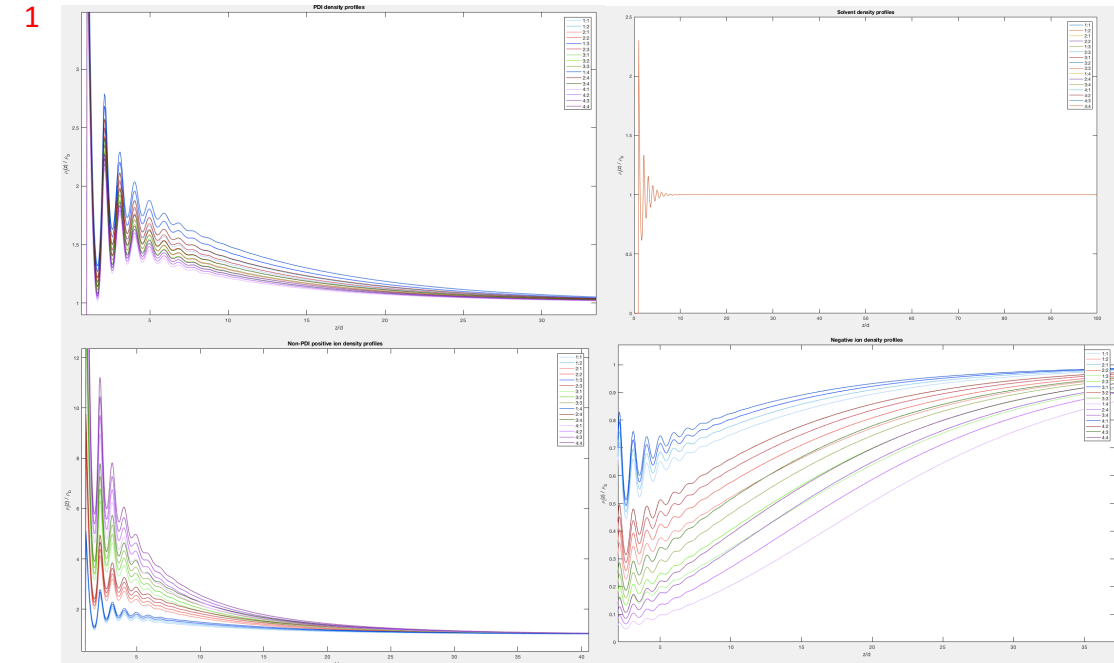
RESULTS: (1) Effect of changing electrolyte valency, (2) Effect of Ionic Strength on Surface Charge, and (3) Effect of Non-electrostatic forces on Surface Charge

APPROACH:

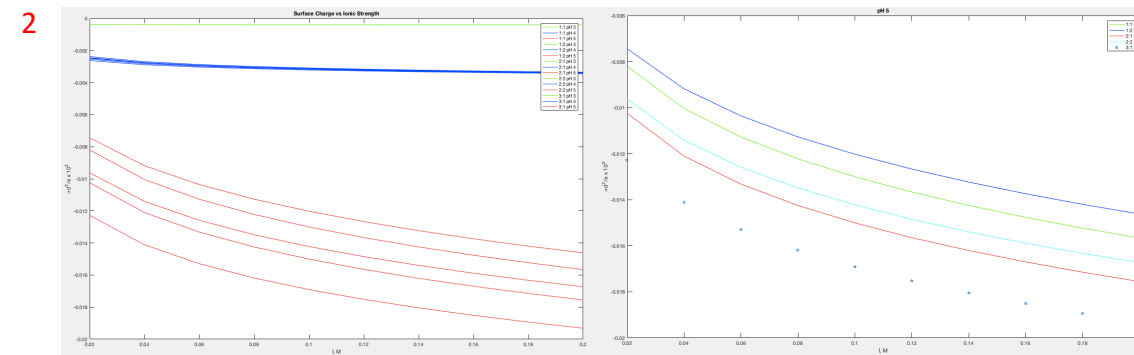
- Surface with a negative charge is assumed
- Consider civilized model with solvent structure and species interactions with one another and the wall considered
 - Species: Potential-determining ions (PDIs), solvent, non-PDI positive ion, negative ion
- Employ charge-regulation boundary condition
- Utilize Classical Density Functional Theory (cDFT) through Tramonto code to minimize the Grand Thermodynamic Potential Functional
- Vary a combination of parameters including: valency of the electrolyte in solution, ionic strength, Leonard Jones component
- Observe species distributions as well as the effect of changing parameters on surface charge

FUTURE WORK:

- Effects of solvation on surface charge in the presence of multivalent electrolytes
- Investigation of surface forces by varying separation distances between two charge-regulating surfaces confining a multivalent electrolyte solution
- Differential capacitance of the double layer in the presence of multivalent electrolytes



- 1
- Varying electrolyte valency minimally affects solvent density
 - Varying positive electrolyte valency increases density of positive electrolyte and banding by valency can be observed, also seen with negative electrolyte
 - PDIs affected by both negative & positive ions, and are more complex



- 2
- Increasing ionic strength of the electrolyte causes more negative surface charge
 - Increasing pH, or decreasing PDI concentration, causes more negative surface charge

- 3
- Hypothesis of increased valency causing a more rapid dissociation was incorrect
 - Increased positive valency causes a gradient

