Coupling of Charge Regulation and Geometry in Soft Ionizable Molecular Assemblies

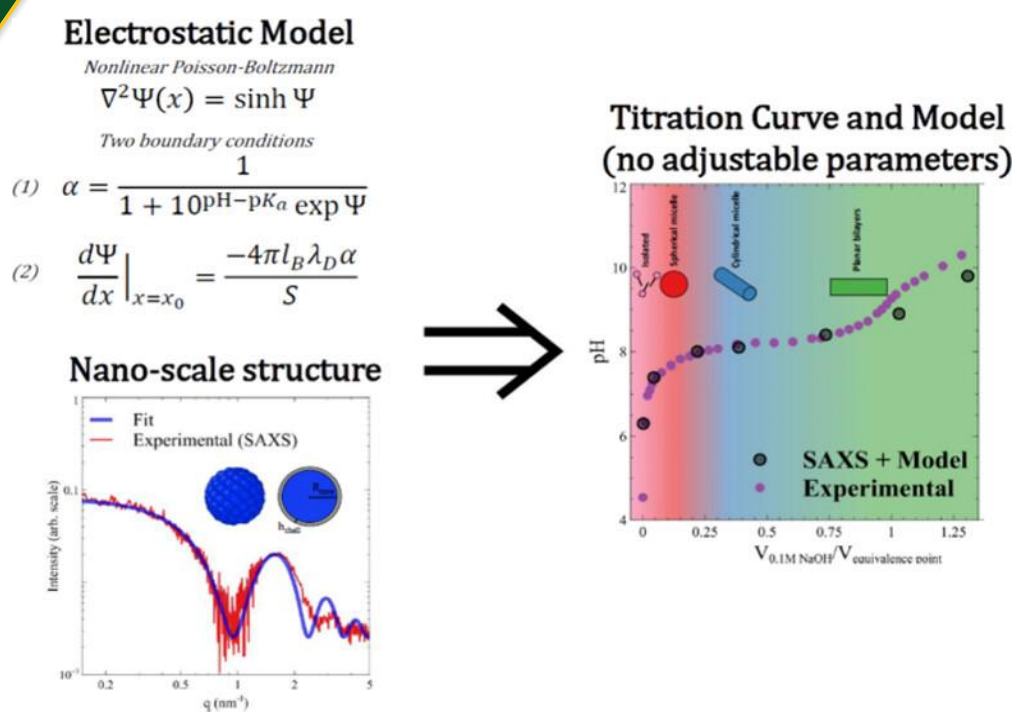

Figure: The theoretical model with its corresponding boundary conditions, along with the particle structures, allows the phase diagram to be determined as a function of pH.

Scientific Achievement

The development of a predictive, parameter-free framework that links molecular charge regulation to self-assembled geometry and environmental conditions.

Significance and Impact

The titration curves and effective charge states demonstrate that pK shifts arise naturally from the coupling between geometry and electrostatics, providing a broadly applicable and physically grounded framework for understanding soft, ionizable materials.

Research Details

- By combining small-angle X-ray scattering experiments with nonlinear electrostatic modeling and simulations, the study shows that structural transitions (e.g., from spherical micelles to cylinders to bilayers) are tightly coupled to ionization behavior.

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