Charge regulation effects on colloidal mixture nanoparticles

Scientific Achievement

This study demonstrates how pH-dependent charge regulation significantly alters the phase behavior and connectivity of colloidal systems.

Significance and Impact

This study shows how pH-driven charge regulation alters self-assembly and suppresses percolation in colloidal systems. By modeling the charge regulation, we improve predictions of material behavior and guides the design of functional nanoparticles with tunable conductivity for applications in energy storage, sensing, and advanced manufacturing like 3D printing.

Research Details

- Hybrid Monte Carlo–Molecular Dynamics simulations are used in a semi-grand canonical ensemble to allow proton exchange between the reservoir and system, enabling realistic charge regulation on particle surfaces
- The study enable more accurate predictions of material behavior and inform the design of functional nanoparticle systems with tunable conductivity—critical for applications in energy storage, sensing, and 3D printing technologies.

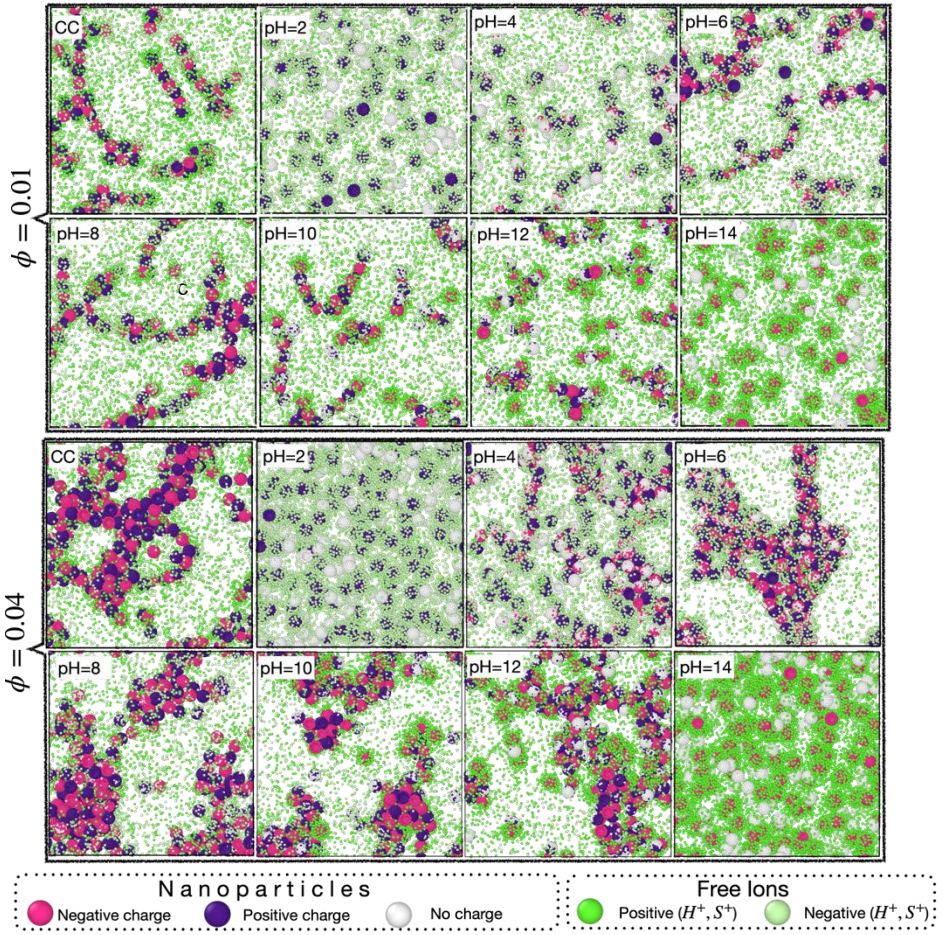

Figure: Schematic representation of the system for an equimolar binary mixture of spherical nanoparticles at ϕ= 0.01 (top set of six panels) and ϕ= 0.04 (lower set of six panels) at different pH values: the first panel of both ϕ= 0.01 and ϕ= 0.04 is a schematic representation of nanoparticles with constant charge (CC), while the subsequent panels correspond to systems with ionizable sites (CR).

Northwestern

Leticia Lopez Flores and Monica Olvera de la Cruz, Accepted in JCP, (2025).