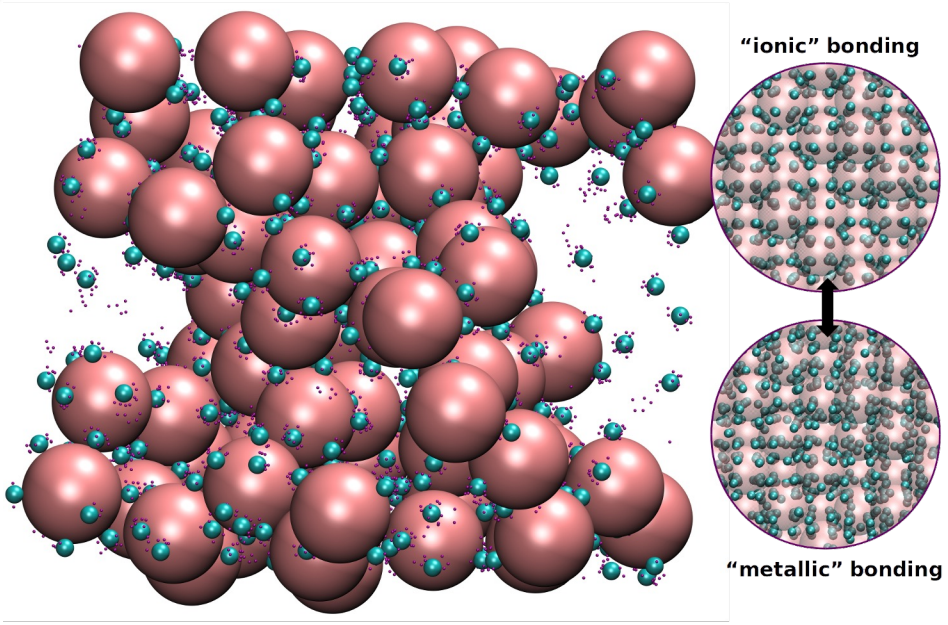
Superionics in Colloidal Crystals



Increase of temperature and nanoparticle concentration in the reservoir change the bonding in the assemblies from ionic-like to metallic-like.

Lin, Y., & Olvera de la Cruz, M. (2022). Superionic Colloidal Crystals: Ionic to Metallic Bonding Transitions.
JPCB 126(35), 6740-6749. DOI: 10.1021/acs.jpcb.2c04041
Work was performed at Northwestern University

Scientific Achievement

Crystal of asymmetric in size oppositely charged nanoparticles (NP) in equilibrium with a reservoir undergo ionic to metallic bonding transition where the small NP lattice melts and the crystals expands.

Significance and Impact

Provides insights on how to control the superionic transition and the crystal structure of charged nanoparticles via temperature and solution composition.

Research Details

- Molecular dynamics simulations are used to study the equilibrium between a binary charged colloidal crystal with a particle reservoir using explicit ions and Coulomb interactions
- Theory based on free energy calculations predicts a phase diagram of colloidal crystals in good match with simulations
- Theoretical analysis reveals the driving force for metallic bonding transition to be enthalpic