

# Charge-driven collapse of nano-cages

Long-range nature of electrostatic forces can have profound effects on the shape and properties of nano-size elastic containers, like nanocages. Due to their small size, electrostatic interaction is strong over distances comparable to the cage radius and can lead to drastic changes of the shape, including the total collapse of the structure. Using Monte Carlo simulations, we demonstrate that small charged nanocages can undergo reversible changes of shapes by modifying the ionic conditions including salt concentration, pH, and dielectric permittivity of the medium. We analyze structures with various charge stoichiometric ratios. At zero or low charge densities, the shape of the cage is determined by its elastic properties, and the surface charge pattern is dictated by the globally fixed geometry. As the charge density per molecule increases, the shape is strongly affected by the electrostatic forces. In this regime, the shape of the nanocage is controlled by the charge distribution.

**R. Sknepnek, G. Vernizzi, M. Olvera de la Cruz**  
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