

# How and Why Highly-Charged Polyoxometalates and Other Highly-Charged Polyions with Univalent Counterions Spontaneously Form Spherical Shells in Dilute Solution

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In 1992, Tianbo Liu demonstrated that aggregates of highly charged polyoxometalates were in fact spherical shells of the type previously known for micelles, liposomes, vesicles, and viruses. In a series of subsequent publications, he further demonstrated that a wide variety of other highly charged polyions spontaneously form spherical shells in dilute solution, including coordination cages, polysilicates, and nanoparticles, regardless of their size and shape.

The question of how and why these spherical shells form has been problematic, since counterion-mediated, short range attraction between ions is known to yield clusters, not spherical shells. I will present an alternative model based on short range repulsion and long range attraction that can account for the stability of these spherical shells. Molecular dynamics simulations provide insight into how the spherical shells are formed in this fashion, and Poisson-Boltzmann calculations provide a theoretical basis for understanding this novel phenomenon.