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Self-assembly of Spherical Macroions in Solution: A Coarse-grained Molecular Dynamics Study[1] ZHUONAN LIU, TIANBO LIU, MESFIN TSIGE, University of Akron, Department of Polymer Science, Akron, Ohio — Macroions (such as polyoxometalates) in solution can form a stable hollow spherical super-molecular structure called blackberry when they have moderate surface charge density and size (1-10 nm). Depending on the surface charge density of macroions, the size of the blackberry can be from 20 to more than 100 nm. Other macroions such as dendrimers can also self-assemble into similar super-molecular structure in solution. Existing theories such as Debye-Hückel and DLVO theories cannot explain this phenomenon and we are not aware of any other theory that can explain this. Previous studies using all-atom Molecular Dynamics simulations have shown identical macroions forming oligomers mediated by counterions. Due to the limitations in all-atom simulation and available computational capabilities, these studies handled only small systems with simple macroions, leading to less conclusive but still relevant results on the self-assembly behavior. To overcome these limitations, in this work large-scale coarse-grained modeling of macroions in solution is used. In order to understand the origin of the attractive force that is responsible for the self-assembly of macroions, different types of macroions in different solution conditions are studied.

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