

## **431f The Effect of Terminal Group Modification on the Solution Properties of Dendrimers: a Molecular Dynamics Simulation Study**

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Dendrimers are large, globular macromolecules that have a regular and highly branched structure. Due to their precise architecture dendrimers can be considered synthetic analogs to proteins. They are able to encapsulate smaller molecules, which makes them appealing for applications in drug delivery. A dendrimer has a large number of terminal groups that can be functionalized to tune its properties. For example, hydrophilic terminal groups can be used to solubilize hydrophobic dendrimers in water or bioactive terminal groups can be used for targeted delivery applications. We have completed molecular dynamics simulations to better understand the conformational changes that variations in terminal group type and arrangement impart to the dendrimer. We will present simulation results for a coarse-grained model of a dendrimer in dilute solution, where the interior repeat units are solvophobic and the terminal groups are varied systematically from all solvophobic to all solvophilic. We will discuss how the size, shape, and mobility of the dendrimer and its parts change according to the fraction and arrangement of the two types of terminal groups.