

Abstract Submitted  
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**The Structure-Function Relationship of PAMAM Dendrimers as Robust Oil Dispersants** BO WANG, NICHOLAS GEITNER, RACHEL ANDORFER, DAVID LADNER, PUCHUN KE, FENG DING, Clemson Univ — Dendrimers are well-defined fractal-like polymers with a hydrophilic surface and hydrophobic interior. Their encapsulation capacity enables biomedical applications such as drug or gene delivery. Recently, PAMAM (polyamidoamine) dendrimers have also been explored as efficient and biocompatible oil dispersants for oil spill remediation. However, their high cationic surface charge has been shown to be cytotoxic. It is therefore imperative to mitigate cationic charge-induced toxicity. Synergistic experimental approach was performed to examine the effects of varying terminal surface charge on the capacity of dendrimers to disperse model linear, polycyclic aromatic, and hybrid hydrocarbons. The discrete molecular dynamics (DMD) simulations with a new MEDUSA force field were also applied to study PAMAM structure and dynamics. We validated our DMD methods by benchmarking against previous experimental and computational results. Our study indicates that uncharged dendrimers collapse by forming intra-molecular hydrogen bonds, which reduce the hosting capability. On the other hand, changing the surface charges from positive to negative greatly shifts the pKa of tertiary amines of the PAMAM dendrimer interior. As a result, the negatively charged dendrimers have a significant percentage of tertiary amines protonated,  $\sim 30\%$ . This unexpected change in interior protonation state cause electrostatic interactions with the anionic terminal groups, leading to contraction and a marked decrease in hydrocarbon hosting capacity.

Bo Wang  
Clemson Univ

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