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Dendrimer – Guest Interactions: Challenging Conventional Wisdom

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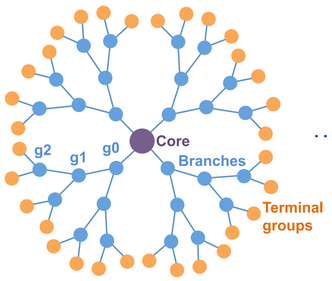
Abstract

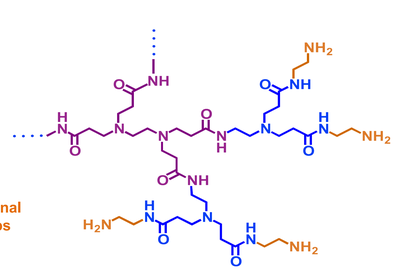
Solutions to many future challenges - including water purification, drug delivery, and energy storage - will require innovative new materials. Dendrimers are a class of materials with wide-ranging applications whose behavior is not fully understood. In many potential applications, dendrimers interact with small molecules. Our work focuses on describing the fundamental mechanisms governing the interactions between dendrimers and hydrocarbons using molecular modeling and computer simulations. A common view of dendrimer host-guest interactions is that the guest molecules are encapsulated in protected interior voids within the dendrimer structure. Our results present an alternative picture and show that the association of a model aromatic hydrocarbon, naphthalene (NPH), involves temporary pockets formed by the dendrimer branches and interactions between the NPH molecules themselves.

Overview of Dendrimers

Dendrimers are three dimensional branched macromolecules comprising a central core, branches of repeating units that define their generation, and terminal groups.



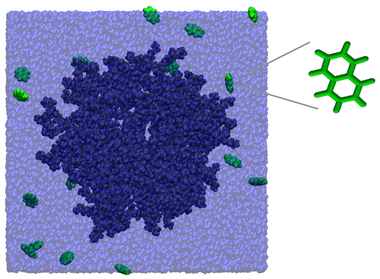
Schematic of dendrimer



Structure of PAMAM dendrimer

Molecular Simulation of Dendrimers

- Molecular dynamics simulations
- 3rd - 6th generation PAMAM dendrimer, 10-17 NPH, explicit water
- NPH:water ratio constant
- OPLS-AA force field
- TIP3P water model
- System size: 72,637 – 131,747 atoms
- Length of simulation: 50 ns
- Ensemble: NpT – 300 K, 1 bar
- Software: GROMACS

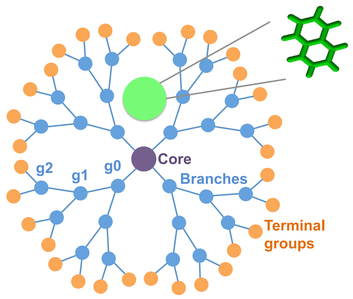


Starting configuration of the G5 PAMAM dendrimer-NPH-water simulations.

Palmetto Supercomputer

Acknowledgments: Palmetto Supercomputing @ Clemson, Dr. Pu Chun Ke, Dr. Ding, Dr. Nick Geitner and Dr. Priyanka Bhattacharya – our experimental collaborators.

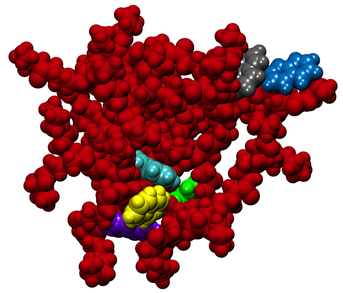
How do small aromatic hydrocarbons associate with dendrimers?



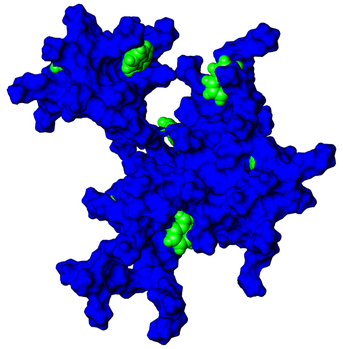
Conventional wisdom:
Small molecules sit in protected voids of the PAMAM dendrimers

What do simulations reveal?

More than just static voids contribute to the association

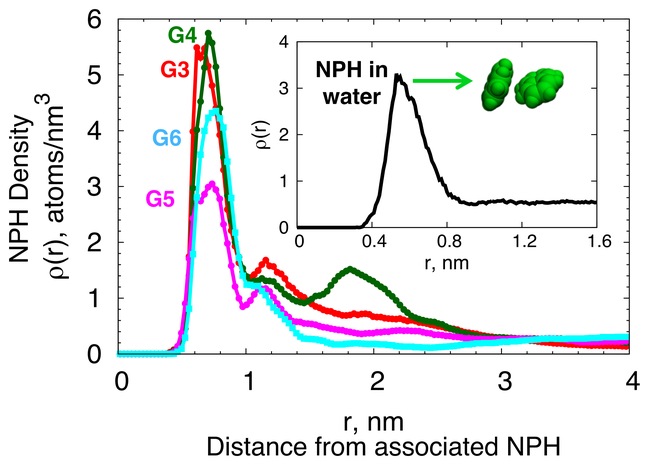


Interactions between associating molecules



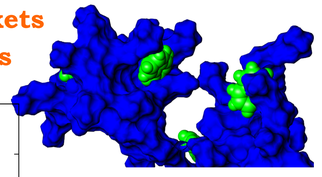
Association sites which reduce water in NPH hydration shell

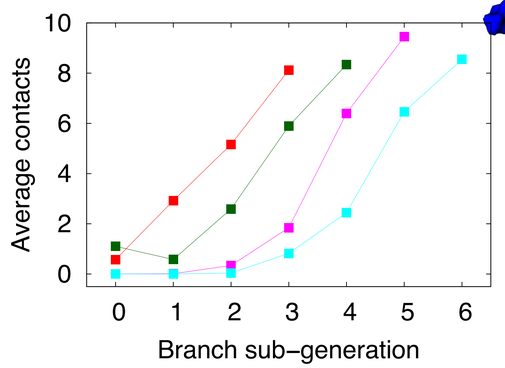
NPH – NPH interactions promote association



- G3 and G4 dendrimers show increased NPH-NPH interactions
- Open dendrimer structure facilitates NPH-NPH interactions

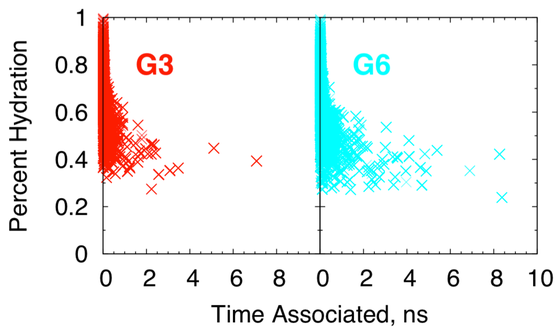
NPH molecules associate in pockets created by dendrimer branches





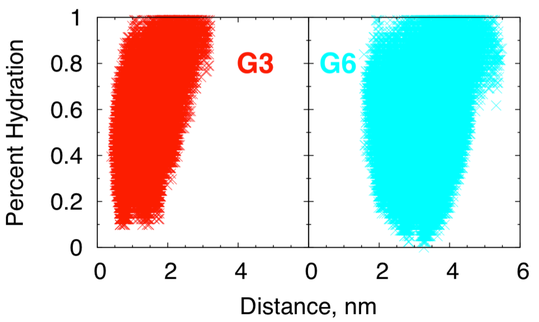
The pockets are mostly formed by the outer generation branches of the dendrimer

Some dehydration rather than interior voids is required for association



NPH molecules that have their hydration shell dehydrated by about 50% remain associated for more than 2 ns

NPH molecules close to the dendrimer center are no more dehydrated than those in the middle regions of the dendrimer



Conclusions and Future Work

NPH association with dendrimers is assisted by favorable interactions between the naphthalene molecules themselves.

NPH molecules associate in pockets which reduce the number of waters in their first hydration shell by about 50%.

- Concentration dependent studies to determine saturation behavior
- Coarse-grained studies of PAMAM dendrimers to examine linear hydrocarbon-dendrimer interactions
- Simulations of hydrocarbon-hyperbranched poly(ethyleneimine) systems.