The MSC-Howard University Collaborative Research Program in Nanoscale Environmental Science and Technology: Overview of Recent Advances

By

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The Materials and Process Simulation Center (MSC) of the Beckman Institute of the California Institute of Technology and the Department of Civil Engineering at Howard University have established a collaborative research program in the emerging field of Nanoscale Environmental Science and Technology (NEST). This program has received funding from the National Science Foundation, the Environmental Protection Agency, the Department of Energy, the Department of Commerce, the NSF Sponsored Cornell University Nanobiotechnology Center, the W. M. Keck Foundation and the National Water Research Institute. Its overall objectives of this research program are to:

1. Characterize the structures and functions of environmentally relevant abiotic/biotic macromolecules, nanoparticles and colloids;
2. Develop and evaluate functional nanomaterials for purification of water contaminated by mixtures of organic/inorganic pollutants, radionuclides and biological contaminants; and
3. Develop and validate quantitative tools for assessing the environmental impact and toxicity of nanomaterials.

This presentation will give an overview of recent advances in NEST with a particular emphasis on the (i) experimental characterization and modeling of proton and metal ion binding to dendritic nanoscale chelating in aqueous solutions and (ii) the recovery of valuable and toxic metal ions from aqueous solutions by dendrimer-enhanced ultrafiltration.

Figure 1: The Multi-Scale Approach for Modeling Proton Binding to PAMAM Dendrimers.

- Continuum Theory
  - Statistical Thermodynamics: Calculation of intrinsic pKa’s of dendrimer ionizable groups
  - Continuum Electrostatics: Calculation of the electrostatic energy of a given charging configuration by solution of the Poisson-Boltzman equation on a grid of collocation points constructed using the 3-D structures from MD simulations

- MD Simulations
  - Equilibrated 3-D structures of dendrimers in water
  - Dendrimer dielectric constant in water
  - Calculation of dendrimer titration curves from averaging over all (or most probable) charging configurations
  - ab-initio DFT: Calculation of intrinsic pH of dendrimer ionizable groups

- Time
  - years
  - 10^-15 seconds

- Distance
  - angstrom
  - nanometers
  - kilometers

Figure 2: Mechanisms Cu(II) Binding to EDA Core Gx-NH₂ PAMAM Dendrimers in Aqueous Solutions. Derived by Combination of EXAFS, EPR and MD Simulations of Water Penetration Inside PAMAM Dendrimers