Monte Carlo simulation study of self-assembly of nanoparticles on Cayley trees CONAN ZHAO, ERIC SCHWEN, ANDREW SEREDINSKI, VINCENT KIM, BRIAN SIMPSON, WILLIAM BANKS, JONATHAN COOK, DAN MAZILU, IRINA MAZILU, Washington & Lee Univ — We present analytical and computational results for a cooperative sequential model with evaporation on general Cayley trees. In particular, we focus on the time dependence of the particle density for a wide range of parameters, such as attachment and detachment rates, tree coordination number, initial and boundary conditions. The model proposed can be used for the modeling of drug encapsulation of nanoparticles using synthetic polymers known as dendrimers, and well as ionic self-assembly of nanoparticles to create optical coatings. Computational results for silica optical coatings using the Ionic Self-Assembled Monolayer (ISAM) technique were compared with experimental results.

Conan Zhao
Washington & Lee Univ