Simulating self-assembly of porphyrin nanorods GREGORY K. GUTHE, ADAM V. SUBHAS, WALTER F. SMITH, JOSHUA SCHRIER, Haverford College — Diacid meso-tetra(4-sulfonatophenyl)porphine (TPPS$_2^{-}$) monomers have been shown to self assemble into nanorods with well-defined cross-section$^1$ and intriguing photoelectronic properties$^2$. However, the structure and conduction mechanism of these nanorods is poorly understood, and questions remain about the aggregation process. Using density functional theory (DFT), we first obtain optimized geometries and atomic-charges for the monomers, which we then use for subsequent molecular dynamics (MD) simulations to observe the initial stages of the self-assembly process. This work uses the resources of the National Energy Research Scientific Computing Center. $^1$A.D. Schwab et al., J. Phys. Chem. B 107, 11339 (2003). $^2$A.D. Schwab et al., Nano Letters 4, 1261 (2004).