Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

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 ($TPPS_4^{2-}$) 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).

Walter F. Smith
Haverford College

Date submitted: 21 Nov 2008 Electronic form version 1.4