Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Calculations of the structural, electronic and transport properties of self-assembled monolayers of porphyrins on the Si(001) surface FILIPE J. RIBEIRO, W. LU, J. BERNHOLC, North Carolina State University — Self-assembled monolayers (SAMs) of organic molecules on surfaces have very promising technological applications. The oxidation states of porphyrins are currently being explored to store charge in a controllable way, aiming at the development of multi-state molecular memories. We present the results of theoretical calculations on the structural, electronic and transport properties of chemisorbed porphyrins on a hydrogen-passivated Si(001) surface. Density-functional calculations were performed to optimize the structural parameters of the adsorbed porphyrins using a real-space multi-grid approach. Electron transport properties for a porphyrin molecule attached to two Si(001) leads were calculated using a non-equilibrium Green's function method in a basis of optimally localized orbitals. Our results show that the current, negligible at low voltages, exhibits a very strong non-linear behavior for bias voltages above 1.5 V, including multiple regions of negative differential resistance (NDR). The multiple NDRs may lead to multi-state molecular devices.

Filipe J. Ribeiro
North Carolina State University

Date submitted: 19 Dec 2005 Electronic form version 1.4