

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Porphyrin-like defects in CN_x nanotubes¹ ANTONIO J.R. DA SILVA, Physics Institute - USP, JAMES ALMEIDA, A.R. ROCHA, Centro de Ciências Naturais e Humanas, UFABC, A. FAZZIO, Physics Institute - USP — Carbon nanotubes (CNT) can be used in a variety of nanoscopic electronic devices, and their functionality can be greatly enhanced by the introduction of defects. It has been shown that CNTs doped with nitrogen atoms can act as sensors. Pyridine-like defects, where four N atoms surround a divacancy, have been shown [1] to act as binding sites of molecules, such as ammonia, and to be associated with the behavior of these sensors. In this work we study the adsorption of iron atoms onto these nitrogen defects. We demonstrate that the Fe atoms bind to the four N defect in a configuration similar to a porphyrin molecule. Moreover, this system - CN_x nanotube plus iron atom - has a magnetic moment of $3 \mu_B$ which is almost entirely localized on the Fe atom. With a combination of density functional theory and recursive Green's functions calculations we study the transport properties of disordered one-dimensional systems [1] composed of such units. In particular, we study the polarization of the current as a function of the average spin orientation of iron atoms randomly dispersed over the nanotubes in a realistic setup. [1] A. R. Rocha, M. Rossi, A. Fazzio and A. J. R. da Silva, Phys. Rev. Lett. **100**, 176803 (2008).

¹We acknowledge support from FAPESP and CNPq.

Antonio J. R. da Silva
Physics Institute - USP

Date submitted: 09 Dec 2008

Electronic form version 1.4