Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Magnetism of Fe double wires deposited on Ir(100) RICCARDO MAZZARELLO, SISSA, Trieste, Italy, ANDREA DAL CORSO, SISSA and DEMOCRITOS-INFM, Trieste, Italy, ERIO TOSATTI, SISSA, ICTP and DEMOCRITOS-INFM, Trieste, Italy — Bulk bcc Fe is a prototypical ferromagnet (FM), but a single monolayer of Fe on W(001) has been known to be antiferromagnetic (AFM). Very recent spin-polarized STM experiments on Fe double chains deposited on Ir(100) 5x1 [1] showed that these adsorbed nanowires are AFM too [2]. We study the magnetic properties of this system using ab-initio density functional theory and both scalar-relativistic and fully-relativistic ultrasoft pseudo-potentials. In particular, we address the energetics of FM and AFM configurations of several experimentally relevant structures. The AFM configuration is always energetically favored, which is in agreement with experiment but does not yet allow to distinguish between different structures. Investigation of the magnetic anisotropy induced by the spin-orbit interaction is in progress. [1] L. Hammer, W. Meier, A. Schmidt, and K. Heinz, Phys. Rev. 67, 125422 (2003). [2] R. Wiesendanger, private communication.

Riccardo Mazzarello
SISSA, Trieste, Italy

Date submitted: 14 Nov 2007 Electronic form version 1.4