Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Magnetic phenomena, spin orbit effects, and electron transport in Pt nanowire contacts ALEXANDER SMOGUNOV, SISSA, Democritos, ICTP, ANDREA DAL CORSO, SISSA, Democritos, ERIO TOSATTI, SISSA, Democritos, ICTP — We present a first-principles DFT study of the electronic, magnetic, and transport properties of short monatomic Pt nanowire contacts. For an infinite tipless Pt wire a fully relativistic calculation, including spin-orbit effects, yields a ferromagnetic ground state already for the unstressed wire [1]. We found that short 3-atom and 5-atom stressed wires in contact with nonmagnetic Pt leads remain locally magnetic, with the magnetization parallel to the wire axis, owing to orbital magnetism. Ballistic conductance of these nanocontacts is calculated using the scattering-based method [2]. Preliminary results indicate a ballistic conductance for a stressed 5-atom wire of about 2.0 G_0 ($G_0 = 2e^2/h$ is the conductance quantum) for parallel magnetization, 2.3 G_0 for perpendicular magnetization, and 2.4 G_0 in the nonmagnetic case. The former is in closest agreement with experimental values reported in break junctions [3].
[1] A. Delin and E. Tosatti, Phys. Rev. B **68**, 144434 (2003); R. Weht, A. Smogunov, A. Delin, A. Dal Corso, and E. Tosatti, in preparation.
[2] A. Smogunov, A. Dal Corso, and E. Tosatti, Phys. Rev. B **70**, 045417 (2004); A. Dal Corso, A. Smogunov, and E. Tosatti, Phys. Rev. B **74**, 045429 (2006).
[3] R.H.M. Smit *et al.*, Phys. Rev. Lett. **87**, 266102 (2001).

Alexander Smogunov
SISSA, Democritos, ICTP

Date submitted: 17 Nov 2006 Electronic form version 1.4