

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Spin-dependent electronic structure of transition-metal atomic chains adsorbed on single-wall carbon nanotubes ENGIN DURGUN, SALIM CIRACI, Department of Physics Bilkent University Ankara Turkey — We present a systematic study of the electronic and magnetic properties of transition-metal (TM) atomic chains adsorbed on the zigzag single-wall carbon nanotubes (SWNTs). We examined the effect of the TM coverage and geometry on the binding energy and the spin polarization at the Fermi level. All those adsorbed chains studied have ferromagnetic ground state, but only their specific types and geometries demonstrated high spin polarization near the Fermi level. Their magnetic moment and binding energy in the ground state display interesting variation with the number of d electrons of the TM atom. Spin-dependent electronic structure becomes discretized when TM atoms are adsorbed on finite segments of SWNTs. Once coupled with nonmagnetic metal electrodes, these magnetic needles or nanomagnets can perform as spin-dependent resonant tunneling devices. Our study is performed by using first-principles pseudopotential plane wave method within spin-polarized density functional method. **Reference:** E. Durgun and S. Ciraci Phys. Rev B 74, 125404 (2006).

Engin Durgun
Department of Physics Bilkent University Ankara Turkey

Date submitted: 20 Nov 2006

Electronic form version 1.4