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The electric and magnetic properties of titanium covered carbon nanotubes SEFA DAG, S. CIRACI, Department of Phyics, Bilkent University, Turkey — We investigated the change of electrical and magnetic properties of Ti coated single-wall carbon nanotubes (SWNT). Our results have been obtained by the first-principles pseudopotential plane wave calculations within density functional theory. We have shown that a semiconducting SWNT can be covered uniformly by titanium atoms and form a complex but regular atomic structure [1]. The circular cross section changes to a square-like form, and the system becomes metallic with high state density at the Fermi level and with high quantum ballistic conductance. Metallicity is induced not only by the metal-metal coupling, but also by the band gap closing of SWNT at the corners of the square. Even more interesting is that uniform titanium covered tubes have magnetic ground state with significant net magnetic moment and the semiconducting tube becomes ferromagnetic metal. However, the magnetic properties of Ti coated tubes depend strongly on the geometry, amount of Ti coverage and also on the elastic deformation of the tube [2]. While the magnetic moment can be pronounced significantly by the positive axial strain, it can decrease dramatically upon the adsorption of additional Ti atoms to those already covering the nanotube. Besides, electronic structure and spin-polarization near the Fermi level can also be modified by radial strain. [1] **S. Dag**, E. Durgun and S. Ciraci, Phys. Rev. B **69**, 121497(R) (2004). [2] **S. Dag** and S. Ciraci, Phys. Rev. B (In press, 2005)

Sefa Dag
Department of Phyics, Bilkent University, Turkey

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