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The physical properties and possible applications of metal coated carbon nanotubes ENGIN DURGUN, Bilkent University, SEFA DAG, ORNL, SALIM CIRACI, Bilkent University — We show that Ti atoms can form a continuous coating of carbon nanotubes at various amounts of coverage. The circular cross section of the tubes changes to a square-like form, and the semiconducting tube becomes a ferromagnetic metal 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. 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. 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 the monolayer coting of the nanotube. Besides, electronic structure and spin- polarization near the Fermi level can also be modified by radial strain. On the other hand, it is found that Ti and V decorated carbon nanotubes of various radii and chirality can adsorb large amounts of hydrogen molecules and can be possible candidates for hydrogen storage applications. The other transtions metals like Fe, Co, Cr, and Mn cannot cover nanotube surface uniformly but can only be adsorbed in clustered forms. Depending on the geometry and amount of adsorption these systems can posses high polarization near Fermi level with variable magnetic moments which can be useful in spintronic devices.

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