Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Electronic and transport properties of carbon-based atomic chain structures R. TUGRUL SENGER, ENGIN DURGUN, Bilkent University, SEFA DAG, Oak Ridge National Laboratory, SEFAATTIN TONGAY, University of Florida, SALIM CIRACI, Bilkent University — Our first-principles calculations show that monatomic chains of carbon have high cohesive energy and axial strength, and are stable even at high temperatures. Pure carbon chains are metallic, and periodic compounds of carbon with transition- metals exhibit half-metallic properties where the electronic spins are fully polarized at the Fermi level. Finite-length carbon atomic chains capped with single transition metal atoms constitute the ultimately small spin-valve systems with high magnetoresistive ratios. In all these structures the electronic, magnetic and transport properties show interesting variations depending on the number of carbon atoms being odd or even.

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Date submitted: 16 Jan 2006 Electronic form version 1.4