

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Half-metallic Silicon Nanowires ENGIN DURGUN, DENIZ CAKIR, NURTEN AKMAN, SALIM CIRACI — This study investigates the atomic structure, mechanical, electronic and magnetic properties of silicon nanowires using first-principles plane wave calculations within density functional theory. We considered bare, hydrogen terminated and transition-metal adsorbed silicon nanowires oriented along [001] direction. Nanowires of different sizes are initially cut from the bulk Si crystal in rod-like forms and subsequently their atomic structures are relaxed. We first presented an extensive analysis of the atomic structure, stability, elastic and electronic properties of bare and hydrogen terminated Si nanowires. The energetics of adsorption and resulting electronic and magnetic properties are examined for different level of transition metal atom coverage. Adsorption of transition metal atoms resulted in magnetic ground state. The net magnetic moment increases with increasing coverage. While specific Si nanowires acquire half-metallic behavior at low coverage, at high coverage ferromagnetic nanowires become metallic for both spin-direction and some of them have very high spin polarization at the Fermi level. Present results are not only of scientific interest, but can also initiate new research on spintronic applications of silicon nanowires. [1]

[1] E.Durgun, D. Cakir, N. Akman and S. Ciraci, Phys. Rev. Lett (2007) (in press).

Engin Durgun

Date submitted: 26 Nov 2007

Electronic form version 1.4