The first major step towards exploiting the spin degree of freedom in electronics was taken in 1988 with the discovery of giant magnetoresistance (GMR) in magnetic multilayered structures. A typical GMR structure consists of a metallic sandwich in which two magnetic layers are separated by a thin, non-magnetic spacer. In this talk I will discuss some molecular systems that show analogous magnetoresistive properties at atomic scales.

Using first-principles density functional theory calculations spin-dependent electronic and transport properties of carbon atomic chains are investigated when they are capped with magnetic transition-metal (TM) atoms like Cr or Co. The magnetic ground state of the TM-C$_n$-TM chains alternates between the ferromagnetic (F) and antiferromagnetic (AF) spin configurations as a function of $n$. The desirable AF state is obtained for only even-$n$ chains with Cr; conversely only odd-$n$ chains with Co have AF ground states. We present a simple tight-binding model that can successfully simulate these variations, and the induced magnetic moments on the carbon atoms. Depending on the relative strengths of the carbon $s$, $p$ and TM $d$ orbital spin-dependent couplings and on the on-site energies of the TM atoms there induces long-range spin polarizations on the carbon atoms which mediate the exchange interaction. When connected to appropriate electrodes these atomic chains display a strong spin-valve effect. Analysis of structural, electronic, and magnetic properties of these atomic chains, as well as the indirect exchange coupling of the TM atoms through the carbon chain will be presented.