Stability and transport of nanocontacts: Ab initio description

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We present ab-initio calculations of the transport properties of the metallic atomic-sized nanocontacts. The nanocontacts were modeled by atomic chains of Co, Fe, Cu, Si, Al separating two semi-infinite magnetic Cu- or Co-leads. The atomic positions of the atoms in the chains were relaxed. Stability of the wires is discussed with respect to the electronic structure of the system. We used the first-principle screened Korrigna-Kohn-Rostoker method to calculate the electronic properties of the systems, treating the leads and atomic chains on the same footing without any model parameters. The Landauer formalism was applied toinvestigate the conductance and magnetoresistance (MR).