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Transport conductivity calculation of atomic-scale nanostructures of Au and Co LIQIN KE, MARK VAN SCHILFGAARDE, Chemical & Materials Engineering Department, Arizona State Univ., PETER BENNETT COLLABORATION — Ballistic transport conductivity calculations on infinite zigzag chains of Co, Au and small-dimension Au nanowires were computed using the Landauer-Buttiker formalism within the full-potential method of muffin-tin orbitals. In the case of infinite zigzag Cobalt chains, one of the two spin channels has quantized transport conductivity. But because of the close spacing of the d levels, the majority channel does not show quantized conductance. In contrast, Au (which are calculated to be not spin polarized) does show well-behaved transport conductivity quantization in the case of infinite zigzag chain. By increasing the dimension of the cross section of the Au Chain, we gradually lose the transport quantization. This is analyzed in terms of a simple model.

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