# *Ab inito* calculations of electron transport through short Au wires with Ag substitutional impurities

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We use a density functional theory (DFT) approach, as implemented in TRANSIESTA package, to calculate electron transport properties of linear gold wires with silver impurities. The wires are attached to two identical bulk gold electrodes with either Au(111) or Au(100) surfaces. We focus our analysis on the dependence of the transmission on the impurity position in the wire. The analysis shows well pronounced transmission oscillations if the wire consists of odd number of atoms. The transmission is enhanced if the impurity occupies even site in the wire, while it is damped for odd sites. These kind of oscillations are suppressed for wires consisting of even numbers of atoms. The result shows that oscillatory behaviour does not depend on surface type. Our *ab initio* findings are explained analytically with the help of a tight-binding model calculations.

9.7 cm

13.4 cm

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