

Abstract Submitted
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Semiconducting chains of gold and silver¹ RICARDO NUNES, FREDERICO FIORAVANTE, Depto de Física - UFMG — The authors introduce a geometry for ultrathin Au and Ag wires that *ab initio* calculations indicate to be more stable than previously considered planar zigzag geometries for these systems, by about 0.1 eV per atom. This structure is insulating for both metals and for related $\text{Ag}_{0.5}\text{Au}_{0.5}$ alloys, with gaps of 1.3 eV for Au, 0.8 eV for Ag, and varying between 0.1 eV and 1.9 eV for the alloys. The insulating nature of the geometry is not a result of Peierls instabilities, and is analyzed in terms of an interplay between geometric and electronic structure effects.

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