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**Oxygen clamps in gold nanowires.** ANTÔNIO J. R. DA SILVA, FREDERICO D. NOVAES, EDWIN HOBI JR., A. FAZZIO, Instituto de Física, Universidade de São Paulo, EDISON Z. DA SILVA, Instituto de Física “Gleb Wataghin”, UNICAMP — We investigate how the insertion of an oxygen atom in an atomically thin gold nanowire can affect its rupture. We find, using *ab initio* total energy density functional theory calculations, that O atoms when inserted in gold nanowires form not only stable but also very strong bonds, in such a way that they can extract atoms from a stable tip, serving in this way as a clamp that could be used to pull a string of gold atoms (see Novaes et al., Phys. Rev. Lett. 2006). In all calculations we have used a GGA-PBE approximation and norm-conserving pseudopotentials. All calculations were performed using the SIESTA code, and we employ a DZP basis function. We observe that the presence of O atoms increases the stability of a local configuration composed of the O atom and its two nearest neighbors at each side (an Au-Au-O-Au-Au structure). This indicates that in an oxygen reach atmosphere it may be possible to pull a longer string of gold atoms (an effect as predicted here has been observed by W. H. A. Thijssen et al., cond-mat/0509376). Finally, local vibrational modes will be investigated.

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