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N and N_2 Enhancing Atomic Chain Formation in Copper Nanowires[1] EDISON Z. DA SILVA, EDGARD P.M. AMORIM, Institute of Physics Gleb Wataghin-UNICAMP- Campinas, SP-Brazil — The trend towards nanominiaturization, with the development of nanodevices, will require the understanding of the behavior of metals at the nanoscale, especially gold and copper. Au and Cu can form very thin nanowires (NWs), as thin as linear atomic chains (LAC). As NWs are produced they can get contaminated. One important question is the effect of light impurities in the mechanical and electronic properties of Cu NWs. We use *ab initio* calculations based in the density functional theory to study the contamination of a linear atomic chain (LAC) of a thin Cu NW with H, C, O, N N_2 and S. In this study we calculate forces before the NW's rupture, binding energies and LAC distances. We show that N and N_2 produce special effects to the LAC as compared with the other impurities. They form strong $p-d$ bonds enhancing LAC formation through rearrangement of tips and inclusion of Cu atoms into the LAC. This effect can be used to produce longer Cu LACs.

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