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Temperature effects in the stability of pure and doped gold nanowires ANTONIO J.R. DA SILVA, Instituto de Fsica - USP Brazil, EDWIN HOBI JR., ADALBERTO FAZZIO, Instituto de Física - USP Brazil — Gold nanowires have attracted a great deal of attention, one of the reasons being the ability to form linear gold chains that are one atom wide and that have just a few atoms in length. One of the amazing characteristics of these wires is their stability, even at ambient temperatures. Therefore, it is very important to understand why they are stable and why they break. Moreover, inserted impurities, such as H and C, can dramatically affect their stability. In the present work we use state-of-the-art ab initio molecular dynamics to perform simulations of pure and doped Au nanowires. We propose a general mechanism that helps to explain the stability of these wires and the rupture process. We show that triplets of Au atoms in the neck of atomically thin nanowires have an instability towards rupture at a length around 6.0-6.1 angstroms. At this length, the potential energy surface (PES) describing the motion of the central atom changes from a single minimum at the middle of the triplet, to a double minimum profile. This provides a consistent picture of the mechanism of rupture of metallic nanowires. Impurities such as C and H also have this behavior. However, as they have stiffer bonds, these PES instabilities always happen in pure Au bonds.

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