Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Ab initio **molecular dynamics study of pure and contaminated gold nanowires** EDWIN HOBI, JR., ANTÔNIO J. R. DA SILVA, FREDERICO D. NOVAES, A. FAZZIO, Instituto de Fí sica, Universidade de São Paulo, CP 66318, 05315-970, São Paulo, SP, Brazil, E. Z. DA SILVA, Instituto de Fí sica "Gleb Wataghin", UNICAMP, CP 6165, 13083-970, Campinas, SP, Brazil — Gold nanowires have the ability to form linear chains that are one atom wide and that have just a few atoms in length. One of the unexpected features of these wires is that before rupture quite large interatomic distances of $\simeq 3.6$ Å have been observed, which are most likely due to the presence of impurities. In view of these facts we recently studied [1] the effect of H, B, C, N, and S impurities on the breaking of Au nanowires, in particular how they affect the maximum Au-Au bond length. Out of all these impurities, under quasi-static pulling conditions the only one that produced an Au-X-Au close to 3.6 Å was hydrogen. All the others produced distances of the order of 3.9 Å or larger. As the calculations were all performed at zero temperature, it is not obvious if, or how, the vibrational motion of the atoms could change these conclusions. In order to investigate these issues we will present results of *ab initio* molecular dynamics for pure and contaminated (H atoms) nanowires. In particular, temperature effects cannot rule out the presence of H atoms in Au nanowires, as recently claimed by Legoas *et al.* [2]. [1] F. D. Novaes *et al.*, Phys. Rev. Lett. **90**, 036101 (2003). [2] S. B. Legoas *et al.* Phys. Rev. Lett. **93**, 216103 (2004). We acknowledge support from FAPESP, Capes and CNPq.

Edwin Hobi, Jr.
Instituto de Fí sica, Universidade de São Paulo, CP 66318, 05315-970, São Paulo, SP, Brazil

Date submitted: 22 Mar 2013 Electronic form version 1.4