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Catalytic Role of Au Nanowires[1] EDISON DA SILVA, ANA PAULA F. NASCIMENTO, Institute of Physics "Gleb Wataghin", UNICAMP, 13083-970, Campinas - SP, Brazil, MIGUEL A. SAN-MIGUEL, Physical Chemistry Department, University of Seville, E41012, Seville, Spain — The oxidation of CO in linear atomic chains (LACs) of Au nanowires (NW) is studied by means of density functional theory calculations using quasi-static (T=0) and finite temperature *ab initio* molecular dynamics simulations. The adsorption of O_2 and CO molecules on the LAC lead to the formation of an intermediate O_2CO complex. Upon thermal activation at room temperature, the complex is able to proceed to oxidation forming a CO_2 molecule and leaving an atomic O impurity into the Au LAC. We report the conditions under which this oxidation pathway takes place. This process also explains the appearance of unusual large Au-Au bond distances in the LAC and attributed to the presence of atomic impurities.

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