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One-dimensional Au chains on TiO_2(110) ADAM KIEJNA, TOMASZ PABISIAK, University of Wroclaw, Poland — One-dimensional (1D) Au chains on the 1×2 missing row (mr) defected, and the added row (ar) reconstructed, TiO_2(110) surfaces are calculated from first principles. Single, dimer, and triple Au rows were considered. The single Au row binds strongly to the mr (2.83 eV) but much weaker to the ar surface (1.56 eV). On the mr surface the bonding of Au is mainly to the Ti atoms below, and to the neighboring Au atoms. In the mr surface the binding energy is decreasing with the number of Au atoms per row, while in the ar surface converse is observed. Even for triple Au rows the binding per atom (2.42 eV) is by 0.17 eV stronger for the mr than for the ar, the latter being suggested as the most favored structure of the clean surface. Thus, Au forms on the 1×2 missing row TiO_2(110) surface strongly adsorbed 1D chains. The charge density distribution and the increased density of occupied states around the Fermi edge suggest metallic behavior of the Au rows. The bonding to the substrate is predominantly covalent. Intra- and inter-chain spacings are determined by the substrate periodicity. The large inter-chain distance (13 Å) on the more or less insulating substrate makes this system ideal for studies of 1D phenomena.

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