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Growth of a gold nanoparticle on TiO_2 surface PABLO DE LA MORA, Facultad de Ciencias, GUSTAVO TAVIZON, Facultad de Quimica, ESTHER AGACINO, Facultad de Estudios Superiores Cuautitlan, Universidad Nacional Autonoma de Mexico — As it is well known gold is very unreactive, but as nanoparticle it has a strong catalytic activity. An Au small cluster is grown in the 110 surface of the TiO_2 with rutile structure. Au atoms are added one by one to the surface, in each step the system is relaxed and different situations are studied. The first Au replaces an oxygen atom that forms a Ti-O-Ti bridge, the removed oxygen bonds to the closest Ti. The objective of this study is to find a cluster with a three dimensional configuration. The system was calculated with the WIEN2k package.

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