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Free gold clusters in CO and O_2 atmosphere: an ab initio study
ELIZABETH C. BERET, LUCA M. GHIRINGHELLI, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin — The marked catalytic activity of gold nanoparticles has inspired a large number of scientific contributions from different fields. However, many questions still lack a satisfying answer, for example what are the structures and stoichiometries of the gold particles in the presence of the reactive gases, and how do their catalytic properties depend on the particle size [1]. We answer these questions for neutral gold clusters modeled in a gas phase atmosphere containing CO and O_2 in variable compositions, and in a temperature range between 100 and 600 K. To this aim, DFT (PBE)–based *ab initio atomistic thermodynamics* technique [2] is applied, including full account of the vibrational contribution to the free energy. As a result, the preferred cluster+adsorbate structures for different environmental conditions are obtained and interpreted as candidate intermediates in the catalytic CO oxidation reaction.

[1] R. Meyer, C. Lemire, S. K. Shaikhutdinov and H. J. Freund, *Gold Bull.* **2004**, *37*, 72–124.
[2] K. Reuter and M. Scheffler, *Phys. Rev. B* **2001**, *65*, 035406; C. M. Weinert and M. Scheffler, *Mat. Sci. Forum* **1986**, **10–12**, 25–30; M. Scheffler and J. Dabrowski, *Phil. Mag. A* **1988**, *58*, 107–121.

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