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On the Oxidation of Palladium clusters supported on alumina/NiAl(110)[1] ROBERTO ROBLES, SHIV N. KHANNA, Dept. of Physics, Virginia Commonwealth University, Richmond, VA 23284 — Palladium nanostructures supported on alumina substrates have been widely studied as catalysts for several combustion processes. Following recent experimental results [1], we have performed electronic structure density functional calculations in order to study the geometry, stability and electronic properties of small Pd clusters supported on alumina/NiAl(110). Using an accurate model of such surface, the properties of selected cluster sizes have been determined, as well as the effect of the addition of oxygen. A carefully analysis of the results as well as a comparison with the experimental data will be presented.

[1] T.Wu et al, Surface Science 603, 2764 (2009).

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