# Ammonia borane dehydrogenation tendencies using Pt4, Au4, and Pt2Au2 clusters as catalysts

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Small metallic clusters -mediated gas phase catalysis studies give lights to understand simple and complex catalytic processes, and help in the discovery and explanation of non-traditional ?molecular-scale? catalytic systems. In this framework and in the context of clean energy sources based on hydrogen, a comparative study about ammonia borane (AB = NH3BH3) dehydrogenation tendencies, using Pt4, Au4, and Pt2Au2 clusters as catalysts, is made. Molecular details on thermal, kinetic (mechanistic) and reactivity factors are revealed. Our results indicate that all the metal tetramers studied here tends to dehydrogenate the ammonia borane molecule, being the processes exothermic, exergonic and fast. Among the studied catalysts, Pt2Au2 shows the best results, because is capable of easily detach several hydrogen atoms, with high probability of taking them out simultaneously, both from B and N, which helps in avoiding the breakage of B?N bond of AB, what is known to produce the poisoning of the catalyst by ammonia generation. 

Ammonia borane

Dehydrogenation

Gold-platinum cluster catalyst

Hydrogen

Theoretical study

Ammonia

Atoms

Binary alloys

Dehydrogenation

Hydrogen

Molecules

Ammonia borane

Catalytic process

Clean energy sources

Comparative studies

Gas phase catalysis

Metallic clusters

Platinum clusters

Theoretical study

Catalyst poisoning