

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Nitrogen and Hydrogen on a Palladium-covered proton conductor: a first principle study of Ammonia catalysis LORENZO PAULATTO, STEFANO DE GIRONCOLI, SISSA, I-34014 Trieste and DEMOCRITOS I-34014 Trieste — Being liquid at ambient conditions Ammonia would be an ideal Hydrogen vector. However, the industrial Haber process for Ammonia synthesis involves high pressures (≈ 100 bar) and temperatures ($450 - 500$ °C), making the process very expensive. Recently, ambient pressure Ammonia production, in the $570 - 750$ °C temperature range, has been reported at the Palladium cathode of a proton conducting cell-reactor [1]. The rate limiting step in the Haber process is N_2 dissociation, while the observed limiting factor in Ref. [1] appears to be the proton transfer through the conductor and it has been proposed that Nitrogen hydrogenation may in this case precede dissociation. We use first-principles techniques to study Nitrogen, Hydrogen and Ammonia interaction with flat and stepped Pd surfaces, in presence of external electric fields. Our aim is to study the effect of electrochemically provided protons on the catalysis of the reaction. [1]G. Marnellos and M. Stoukides, Science 282, 98 (1998); G. Marnellos, S. Zisekas, and M. Stoukides, J. of Catalysis 193, 8087 (2000)

Lorenzo Paulatto
SISSA, I-34014 Trieste and DEMOCRITOS I-34014 Trieste

Date submitted: 26 Nov 2008

Electronic form version 1.4