Surface Science studies of FeS_2 for catalytic N_2 reduction

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Ammonia synthesis is reckoned to account for over 1% of the world´s consumption of man-made power, driven predominantly by the production of fertilizers and pharmaceuticals [1]. Of all the classic catalytic reactions, ammonia synthesis is arguably the instance for which tuning catalytic efficiency is most urgently required. Intriguingly nitrogenase (found in symbiotic and free-living diazotrophs) catalyses the reduction of nitrogen to ammonia, under ambient conditions, in lively contrast with the energy-consuming industrial Haber-Bosch reaction. Efforts of protein crystallography have gradually unveiled that the active site of nitrogenase is essentially a FeS_x nanocluster, with a central light atom and a Mo atom [2,3].

In the light of the above understanding, we decided to investigate the interaction of N_2, H_2 and NH_3 on the surface of naturally grown single crystal FeS_2{100}. The adsorption of nitrogen species was studied using both background dosing and activated N_2 species directed to the pyrite surface [4]. The synthesis of ammonia from hydrogenation of adsorbed nitrogen species was subsequently studied [5]. The gas-surface interactions were investigated under a wide range of conditions to evaluate the particularities of NH_3 synthesis on pyrite single crystals.

References

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