Nitrogen Adsorption and Hydrogenation on a MoFe6S9 Complex

The enzyme nitrogenase catalyzes the biological nitrogen fixation where N-2 is reduced to NH3. Density functional calculations are presented of the bonding and hydrogenation of N-2 on a MoFe6S9 complex constructed to model aspects of the active site of nitrogenase. N-2 is found to bind end on to one of the Fe atoms. A complete energy diagram for the addition of hydrogen to the MoFe6S9 complex with and without N-2 is given, and a mechanism for ammonia synthesis is proposed on this basis.

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