Two-state Reaction Mechanism of the Synthesis of Ammonia in the N2/H2/Ru Systems: A Theoretical Study

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Abstract

Ru-based catalysts show high activity and stability to produce ammonia. Herein, the two-state reaction mechanism of Ru catalyzes N2 and H2 to synthesize NH3 are theoretical studied with the density functional theory(DFT)UB3LYP methods. The spin-orbital coupling constant(Hsoc) and intersystem crossing probability(Pisc) at minimum energy crossing point(MECP) were calculated, respectively. its are: Hsoc,MECP1=508.34cm-1,P2,MECP1ISC=0.85,MECP2:Hsoc,MECP2=269.21cm-1, P2,MECP2ISC=0.27. Used energy span model to determined TOF-determining transition state(TDTS) as 3TS2-3 and TOF-determining intermediate(TDI) as 3IM9 of reaction.In addition, the charge decomposition analysis(CDA), spin population analysis and frontier molecular orbital(FMO) theory were used to analyzed reaction mechanism.

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