XII CBTERMO
VIII ESCOLA DE TERMODINÂMICA
CURITIBA 2024

XII Congresso Brasileiro de Termodinâmica
VIII Escola de Termodinâmica

De 5 a 9 de Maio de 2024
Curitiba - Paraná - Brasil

A DFT investigation of the N_2 reactivity with metallic nanoclusters for enhancing the photocatalytic synthesis of Ammonia

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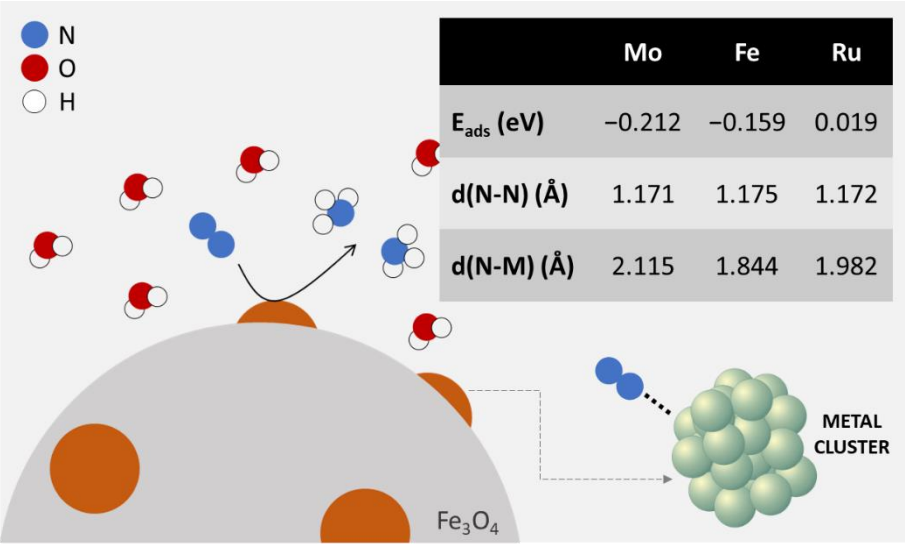
RESUMO GRÁFICO



ABSTRACT

Ammonia has been pitched as one of the most cost-effective alternatives for hydrogen storage and transportation. However, the conventional fabrication of ammonia is both carbon- and energy-intensive, responding for ca. 2% of the overall global carbon emissions and energy consumption. To overcome this conundrum, alternative synthetic routes have been proposed, including photocatalysis. Photocatalysts for the synthesis of ammonia are often doped with metallic nanoclusters to improve their efficiency. In this direction, this work investigates the energetics of nitrogen adsorption and reactivity on different metallic nanoclusters is investigated *in silico* using Generalized Gradient Approximation (GGA) PBE functional. Studies of N_2 and NH_x (x = 0 to 3) interactions with selected surfaces of the clusters were carried

out using the projector-augmented wave (PAW) method implemented in the GPAW package of the Atomistic Simulation Environment (ASE). Partial results show that the nitrogen adsorption energies on distinct metal surfaces are significantly lower compared to a pure magnetite iron oxide (222), indicating a higher affinity potential for enhanced catalytic activity when the clusters are used. Specifically, the adsorption of N_2 on Mo (110) and Fe (110) showed the lowest adsorption energies, at −0.21 and −0.15 eV, respectively. Adsorption on Ru (110) showed a slightly positive E_{ads} = 0.02 eV, being the least favorable cluster investigated. These findings underscore the potential of metallic doping in iron oxide nanoclusters for efficient N_2 adsorption, paving the way for more sustainable and energy-efficient routes for synthesizing ammonia. Detailed analysis and full results will be presented, offering insights into the design of novel catalysts for green ammonia production.

Keywords: DFT, Iron Oxide, Nanoclusters, Ammonia, Adsorption.