

Rational Design of a CuPd Nanoparticle Catalyst for Electrochemical NO_3^- Reduction Using Computational Techniques

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Nitrate (NO_3^-) has become a major pollutant in the biosphere as agriculture and industry have intensified to feed the growing world population[1]. Removing NO_3^- by reducing this species to a less harmful N-containing species is a potential solution.

Reduction of NO_3^- is not a trivial process, due to a multitude of possible reduction products, including molecular nitrogen (N_2), nitrite (NO_2^-), ammonia (NH_3), and nitrous oxide (N_2O). An ideal denitrification catalyst would be selective towards N_2 as it is the most chemically benign of these products. On top of the issue of selectivity is the issue of activity; catalysts must also be active, and display a reaction rate that will not limit the utility of a given catalyst.

One of the most promising catalytic materials for denitrification is a bimetallic CuPd nanoparticle catalyst[2]. CuPd nanoparticles have been observed to have high activity and selectivity for NO_3^- reduction toward N_2 [3, 4]. It has been proposed that this activity/selectivity is due to the presence of a wide range of active sites, with specific sites able to catalyse individual steps of the denitrification process. However, studies have shown conflicting results and no systematic study of CuPd nanoparticles has been done to date.

We are currently undertaking a systematic approach to understand the role of the architecture of the active sites in the activity and selectivity of the CuPd nanoparticle catalyst for NO_3^- reduction using DFT calculations. The present work will address the issue of selectivity, initially on pure Cu and pure Pd, before turning to CuPd bimetallic surfaces. Results thus far will be presented, including insights into the mechanism of formation of various NO_3^- reduction products.

References

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