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Bio-inspired nano-sulfides catalyse the production of organics from CO₂

N.H. DE LEEUW,¹² A. ROLDAN,¹ N. HOLLINGSWORTH²

¹Cardiff University, School of Chemistry, Park Place, Cardiff CF10 3AT, UK

²University College London, Department of Chemistry, 20 Gordon Street, London WC1H 0AJ, UK

In recent years, carbon dioxide capture and utilisation is gaining increasing attention, driven not only by environmental concerns but also by the potential to use it as carbon feedstock for fuels and chemicals. One plausible utilisation route is its conversion to form small organic molecules, yet CO_2 is thermodynamically very stable and its reduction is energy intensive.

One of the most exciting scientific debates involving iron sulfides focusses on their proposed pivotal role in a leading theory on the Origin of Life [1]. The widespread occurrence of iron sulfides at hydrothermal vents as a series of highly reactive metastable compounds have led to their implication as catalysts in the conversion of CO2 to small organic molecules, backed up by their presence as vital redox centres in contemporary enzymes. In chemoautotrophic bacteria CO₂ conversion takes place under mild conditions in catalysed by enzymes. These enzymes often contain Fe₄S₄ clusters, which have been shown to act as electron-transfer sites, but they can also be catalytically active centres for molecule transformations. The iron sulfide mineral greigite is structurally similar to this cluster (Fig. 1) and may therefore be a promising catalyst in CO2 reduction reactions.

Here, we present the results of a combined computational and experimental investigation into the applicability of the greigite mineral (Fe₃S₄) as a catalyst to transform CO_2 into small organic molecules, such as formic acid and methanol.



Figure 1. Schematic representation of (A) the ferredoxin center of the CO dehydrogenase enzyme, (B) greigite surface, Fe_3S_4 (001), with an enhanced cubane structure.

[1] M.J. Russell, W. Martin, *Trends Biochem. Sci.* (2004) **29**, 358.