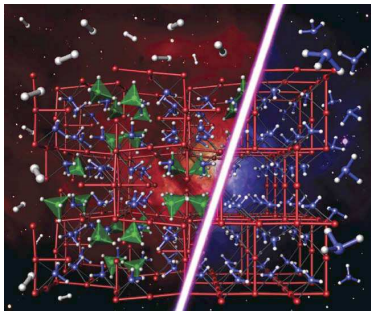
IT Services

Case Study

BlueBEAR provides a substantial computing resource that properly supports the research work of research staff and students at Birmingham. It provides a cost effective facility that optimises the effectiveness of research and ensures the University continues to be a world-class academic learning and research environment.

Biocatalysis for applications in PEM fuel cells



Challenges

To gain a better understanding of the processes involved in producing metallic nanoparticles through biomineralisation processes.

Background

The interest in nanoparticles produced through biomineralisation processes is due to the fact that they can have different properties to nanoparticles produced through other synthesis methods. An important factor in understanding the possible difference in activity is to study the way in which they are formed. This involves studying interactions between growing nanoparticles and the biological molecules that surround them.

Furthermore, biomineralisation has several 'green' properties making it appealing due to the desirability of reducing carbon emissions. Bacteria have been used to produce clean bio-H2 through fermentation processes. The spent biomass can be used to reclaim precious metals, such as those found in catalytic converters, to form nanoparticles. A better understanding of the processes involved in this could aid in producing a cheaper, cleaner hydrogen economy.

Results

Research will focus mainly on modelling nanoparticles produced through biomineralisation processes, looking more specifically at those produced by bacteria. Preliminary work has been focused on computing stable structures of small pure metal (Pd and Pt) and bimetallic (Pd-Pt) clusters, looking at size effects as well as varying composition, utilising DFT as well as coupling genetic algorithm search techniques with empirical potentials. From these early simulations the research will progress towards more complex calculations of the interactions between the metal nanoparticles and biological molecules such as proteins, lipids and carbohydrates. This will give a valuable insight into biomineralisation processes for generating metal nanoparticles and may allow them to be more effectively tailored to catalytic applications, for example in fuel cells.

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Product Used
NWChem
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Genetic Algorithm based programs

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