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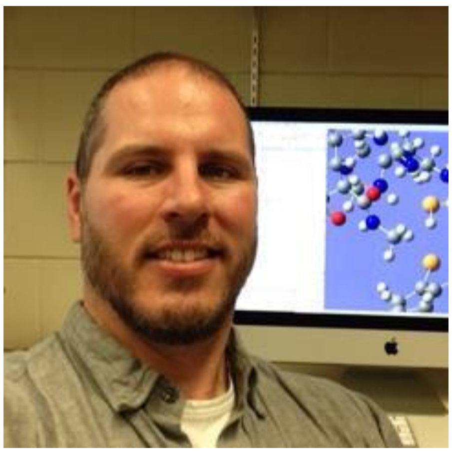
BRANDON UNIVERSITY

RESEARCH CONNECTION

Using computers to solve Earth’s energy problems

By Eric Bushnell, Ph.D.



Why this research is important

Metal-dithiolene complexes (Figure 1) have been investigated for potential use in the purification of olefins used in the production of polymers, dye-sensitized solar cells, photo catalysts for the splitting of H_2O to produce H_2 and more recently as photothermal therapeutic agents for the treatment of cancer.

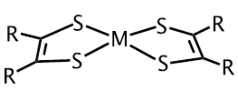


Figure 1: A general metal-dithiolene complex

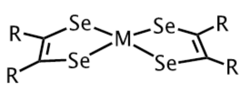


Figure 2: A general metal-diselenolene complex

Given the rich and diverse chemistry of metal-dithiolene complexes, it is not surprising that they are well investigated. However, analogous metal-diselenolene complexes (Figure 2) have not been as well studied.

What you need to know

We are currently investigating metal-diselenolene for their use for the production of H_2(g) to be used in hydrogen fuel cells. Past research in my group has investigated other aspects of the chemistry of such metal-diselenolene complexes and has found subtle differences that make the diselenolene complexes attractive for use in chemical reactions involving the transfer of electrons, such as the production of H_2(g) from water.

Increasing levels of greenhouse gases in our atmosphere threaten our planet as a result of climate change. A main component of greenhouse gases is carbon dioxide and is a primary product of fossil-fuel consumption which is required for the planet's energy demands. In fact, 80% of the world's energy consumption is derived from the burning of fossil fuels. Based on current emission levels of CO_2 into our atmosphere, the Earth is on track for continued global temperature increases. Importantly, it has been stated that an increase of 2 °C in Earth's average temperature is considered a benchmark where the risk of climate change becomes threatening. Based on the current levels of CO_2 emissions, the probability of reaching this 2 °C benchmark by 2100 is 88%! Thus, to prevent this increase of 2 C° urgent action is required. Such action involves reduced fossil fuel consumption and the development of renewable energy sources to reduce the amount of CO_2 emitted into our atmosphere.

Currently, there are several alternative energy sources available such as wind, solar, and tidal. The most viable path for large-scale growth of alternative energy sources involves solar energy conversion and—specifically—the photocatalytic splitting of water to form molecular hydrogen to be used as an alternative fuel. While hydrogen is the most abundant element in the universe, molecular hydrogen itself is not present on earth in significant amounts and must be produced from a hydrogen-containing source, such as water. Electrolysis of water allows for the conversion of electricity into chemical energy, allowing for separation of hydrogen from water. However, presently there are limited methods available for hydrogen fuel production that are efficient and do so at relatively low costs. As a means to minimize costs, research is under way in the development of various catalysts using cheap-metals such as copper, nickel, iron, and cobalt. However, many catalysts previously investigated for the production of molecular hydrogen decompose over time due to the hydrogenation of the ligands.

How the research was conducted

In the research lab, a computational chemistry tool was used, which involves the use of computers to solve the complicated equations of quantum mechanics allowing chemical systems and reactions to be studied at the atomic level. We studied the Ni-bis (1,2-diamine-diselenolene) and Ni-bis(1,2-dicyano-diselenolene) complexes using Density Functional Theory for the renewable production of H_2(g) to be used in hydrogen fuel cells.

What the researchers found

Present results from my research program are promising and suggest that select nickel-diselenolene catalyze the formation of H2(g) with a small energetic cost in a dilute aqueous environment.

How this research can be used

Knowledge gained from this work and ongoing work will provide insight into the design of new catalysts for the renewable production of H_2 via the photocatalytic splitting of water. Moreover, the results from my research may offer solutions to the problems currently faced in the production of H_2 seen in past experimental work.

About the researchers

Eric Bushnell is an assistant professor at Brandon University and teaches courses on thermodynamics, kinetics, electrochemistry, quantum chemistry and computational/theoretical chemistry.
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Keywords

hydrogen evolution reaction; HER catalysts; alternative fuels, diselenolene; density functional theory; nickel-bis(diselenolene)

Publications based on this research

Boychuk, B. T. A., Bushnell, E. A. C. (Forthcoming). A computational investigation into nickel-bis(diselenolene) complexes as potential catalysts for reduction of H+ to H2. *Canadian Journal of Chemistry*.

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