Structural Determination of a Bioinspired Perchlorate Reduction Catalyst Through Chemical Modeling

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Perchlorate, an oxidizer found in rocket fuel and fireworks, has leaked into groundwater near military sites and factories. It's consumption can have major adverse effects on health by disrupting the function of the thyroid gland. Ion-exchange resins designed for the removal of perchlorate must be regenerated, producing a waste brine containing perchlorate that is difficult to dispose of. This perchlorate must be reduced to safer forms, such as chloride, with the aid of catalysts. In my previous project, I developed a catalyst that efficiently reduces perchlorate in the ion-exchange waste brine and outperforms all previous catalysts. However, I found that nitrate acted as a strong inhibitor of the catalyst, which prevents the direct use of the catalyst on waste brine, which contains nitrate. The goal of my current research is to understand why nitrate acts as an inhibitor and further optimize the efficiency of the catalyst. However, this is very difficult without knowing the exact structure of the catalyst. Due to its heterogeneous nature, the catalyst is insoluble in water and most organic solvents, making it impossible to determine the exact structure of the catalyst using single-crystal X-ray diffraction. To overcome this, I devised a computational method to determine the catalyst's structure. I researched literary publications to deduce possible structures of the catalyst and modeled them using the Gaussian software, which runs an algorithm to calculate their single point energies. The lowest energy structure is most probable to be the actual structure of the catalyst. Finding the structure of the catalyst will be a crucial step to achieving my goal: for water industries to implement the catalyst design and decontaminate drinking water nationwide.