Biomimetic modifications of a FeNi Hydrogenase bridging cys residue ligand

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We are studying a FeNi Hydrogenase which can be used to catalyze the conversion of hydrogen to protons and electrons. Using Gaussian 16, a computational chemistry software, we are able to simulate chemistry that one does not necessarily have enough time or resources to do in a laboratory setting. The calculations acquired computationally determine biomimetic modifications that can be made to the native enzyme active site, directing chemists working in the lab towards potentially favorable biomimetic catalysts. Previous research has been conducted on propanedithiol, a common biomimetic ligand, and for my research, I am altering these bridging cys residues. Specifically, based on a similar ligand found in the native FeFe Hydrogenase active site, I replaced the center carbon in the propane with an amine group and optimized the system using a Density Functional Theory method. The information obtained from this will help experimentalists decide if the new ligand is worth testing in their catalysts. Practically, a catalyst with FeNi Hydrogenase properties could be used to sustainably oxidize hydrogen, which would be a great renewable alternative energy source.