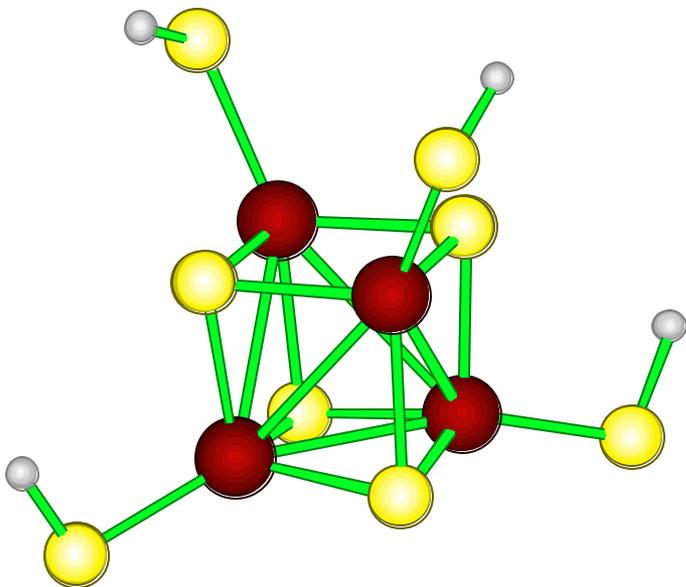


Fe-S Clusters



Fe-S proteins are ubiquitous in living organisms. They belong to one of the most important classes of biological electron transfer agents. Their functionality is critically dependent on the electronic structure of their active sites, i.e. one-Fe center, Fe₂S₂, Fe₃S₄, and Fe₄S₄ clusters.

We reported a combined experimental and theoretical study on the electronic structure and reduction / oxidation energy of one-Fe center. Some preliminary optimized structures of the Fe₄S₄ clusters have been obtained.

The .global minimum structure [Fe₄S₄(SH)₄]²⁻ is shown here.

Reference:

“A Combined Photodetachment Spectroscopy and Computational Study of Reduction Potentials of Rubredoxin Redox Sites”, Shuqiang Niu, Xue-Bin Wang, Jeffrey A. Nichols, Lai-Sheng Wang, and Toshiko Ichiye, *J. Am. Chem. Soc.* submitted.