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## IV.C.1n A Biomimetic Approach to New Adsorptive Hydrogen Storage Metal-Organic Frameworks

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4. In hemoglobin, the oxygen-binding is strengthened by four sub-units working cooperatively. In the new hydrogen storage system, two nets of the new material can be interwoven into one to achieve cooperative binding.
5. The concentration of the active centers in hemoglobin must be high enough to sustain the respiration required for a living organism.

In a similar way, the new hydrogen storage material must contain high density of active metal centers to reach high gravimetric and volumetric hydrogen storage capacities to allow a reasonable driving range.

The new approach includes the design and preparation of large organic molecules containing two levels of anchors, with primary anchors supporting the porous structure and secondary anchors fixing more active metal atoms. The organic molecules will be mixed with metal salts under previously explored conditions to promote interwoven structures and hemoglobin-like metal centers. After removing guest molecules in the metal-organic host, more active metal atoms will be introduced to the host. These active metal atoms will be escorted by chaperon molecules so that the metal atoms will not stick together but be bound individually to the secondary anchors in the metal-organic material to form a hemoglobin-like artificial protein.

### Objectives

The focus of the research is the use of concepts evident in hemoglobin to guide the synthesis of metal-organic materials with suitable hydrogen affinity. The objective is to increase the hydrogen-adsorption heat to reach the DOE storage goals at room temperature and applicable pressures.

### Approach

The approach is inspired by oxygen transport proteins such as hemoglobin, which functions in respiration. The reversible oxygen binding in hemoglobin is analogous to the vehicular hydrogen storage problem in many ways:

1. Both systems switch from taking in to giving out gas molecules by lowering the pressure or raising the temperature.
2. Both contain metal atoms with open binding sites; these sites interact with gas molecules strongly.
3. In both cases, the active metal centers are reactive and require protection from the channels in which they reside. There exist optimum dimensions for the channels so that the surroundings of the metal atoms can also interact with gas molecules.