

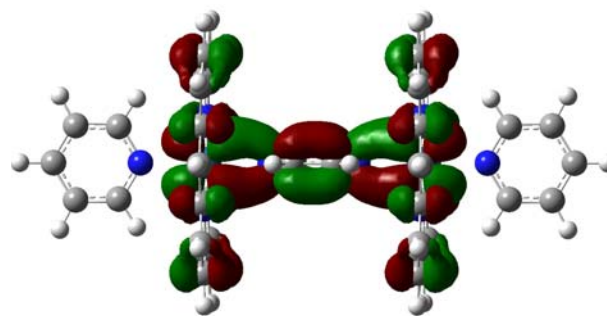
# Electron Transfer in Metalloporphyrin Dimer Systems

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Research Experiences for Undergraduates

Many biological systems contain porphyrin rings that participate in electron transfer reactions. There is a burgeoning interest in the field of nano-technology to use these Porphyrins complexed with metals as molecular devices. Therefore, there is significant interest in understanding the rates of these electron transfer reactions to provide information as to the efficacy of studied systems as molecular devices. The rate of electron transfer is proportional to the square of the magnitude of the electronic coupling element ( $H_{DA}$ ) for weakly interacting systems. Thus, if it is possible to create metalloporphyrin systems that exhibit desired coupling elements, porphyrins could well be on their way to being incorporated in molecular devices.

**Undergraduate Student John Andrew Kouzelos (HMC)** demonstrated the feasibility of obtaining the electronic coupling element using calibrated data from an *Ab initio* computational method on asymmetrical

and symmetrical Metalloporphyrin dimers using the Koopman's Theorem Generalized Mulliken-Hush method. Both Ruthenium and Osmium containing Metalloporphyrin systems with a variety of attached ligands were studied. Results show that asymmetrical systems exhibit coupling elements reminiscent of the average of two analogous symmetrical dimer systems. Findings also suggest that linear Osmium dimers exhibit electronic coupling elements that are larger in magnitude than those of their ruthenium counterparts ( $2087\text{cm}^{-1}$  vs.  $1305\text{cm}^{-1}$ ).



A metalloporphyrin system with coupling orbitals.