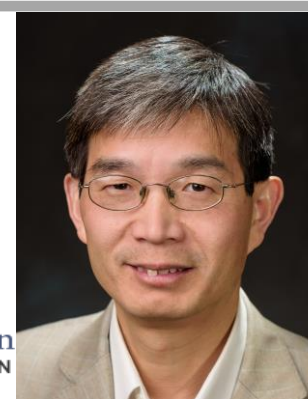


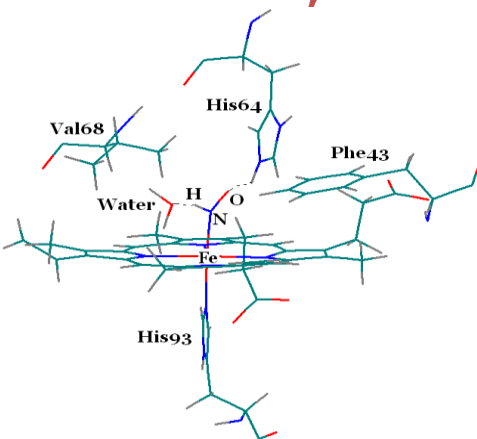
# High Accuracy Computational Chemistry Lab

Dr. Yong Zhang, Department of Chemistry and Chemical Biology

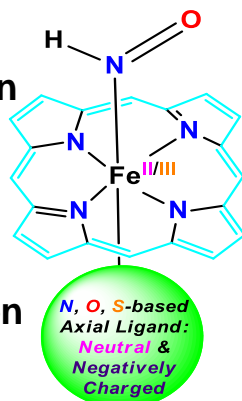
>120 publications, with ~ 1/3 in top journals



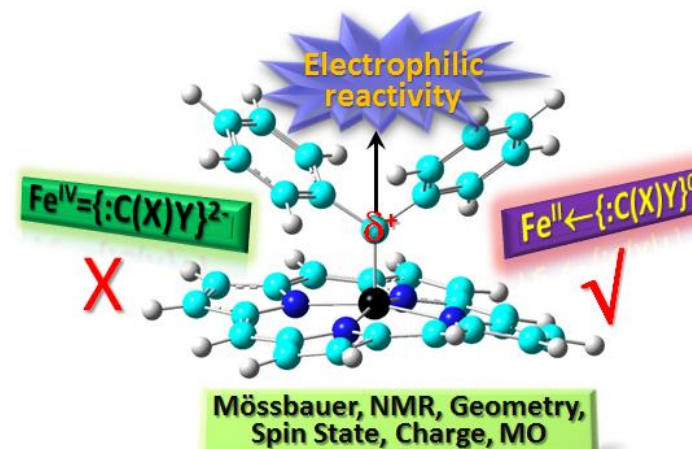
## Metal-mediated biological HNO binding, formation, conversion, and detection



- HNO → cAMP
- More favorable effect than NO to treat heart failure
- Potential treatment for reduction of neuronal damage
- Enzyme activity regulation
- ...

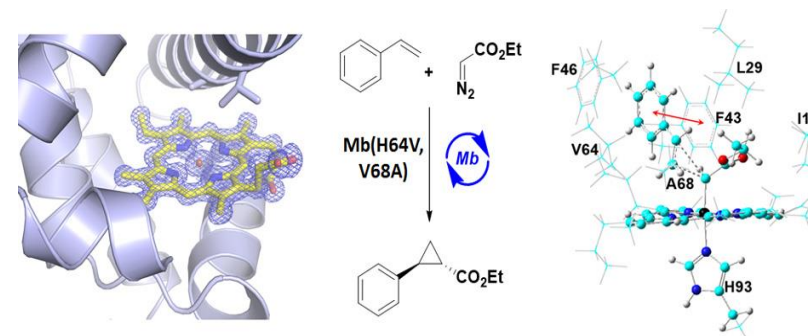
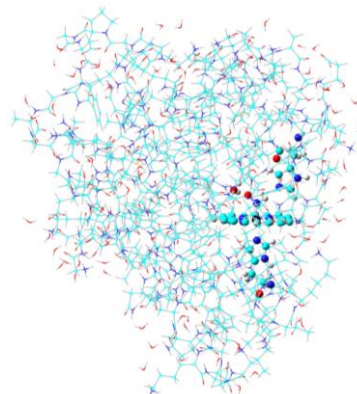
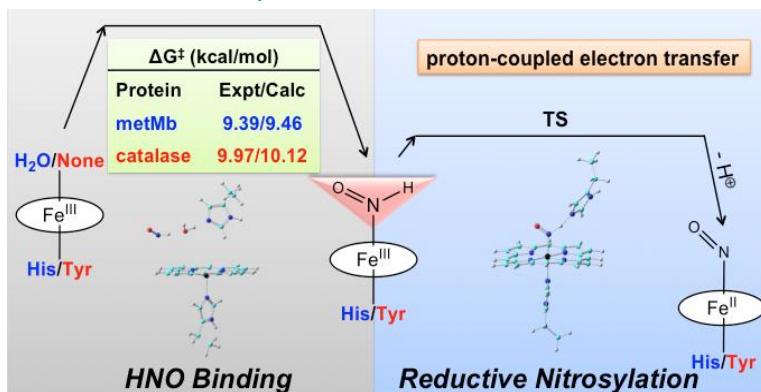


## Sustainable carbene transfer reactions catalyzed by artificial heme proteins & models



- C-H insertions
- N-H insertions
- S-H insertions
- Si-H insertions
- Cyclopropanations
- ...

mechanisms of reactivity, stereoselectivity, and chemoselectivity



One reaction:  
 Expt: 99.9% de; 99.9% ee  
 Calc: 99.9% de; 99.8% ee

Another reaction:  
 Expt: 99% de; 84% ee  
 Calc: 99.9% de; 85% ee