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## **Bc/Master/PhD STUDENTS WANTED!**

### **Please feel free to contact Martin Srnec for more info.**

The project, based on the use of an arsenal of theoretical methods, aims at calculations of redox properties of metalloenzymatic active sites and elucidation of their effects on reactivities and selectivities with respect to a possible design of new catalysts.

Specifically, we offer to work on one of the following topics:

- ✓ Redox vs. acidobasic contributions to H-atom transfer reactivity/selectivity in enzymes and bioinspired complexes
- ✓ Electronic structure contributions to selectivity in mono and binuclear non-heme iron active sites
- ✓ Radical biocatalysis: Physico-chemical factors controlling reactivity and selectivity in SAM radical metalloenzymology