NITRATE/NITRITE SELECTIVITY OF ZN(II) PORPHINE. **Christi W. Young**, William A. Maza, H. Lee Woodcock III, and Randy W. Larsen. Department of Chemistry, University of South Florida, 4202 E. Fowler Ave CHE205, Tampa, FL 33620.

Selectivity of small molecule binding to metalloporphyrins is important for numerous appliations in biology and industry ranging from sensors to highly efficient catalysts. Of specific interest is the selectivity of nitrite/nitrate associated with Zn(II) porphyrins, as this system may serve as a model system for the binding selectivity of Zn-metal clusters towards a wide range of nitrogen oxides. To explain selectivity of nitrite over nitrate by Zn(II)[5,10,15,20-tetraphenyl porphyrin] (ZnTPP), and an increase in affinity for both nitrite and nitrate when pyridine is present as proximal base, the interactions of a model for ZnTPP, Zn(II) Porphine (ZnP), with nitrite, nitrate, and pyridine were examined using with Density Functional Theory (DFT). The preference of nitrite binding is rationalized through the metal-to-ligand orbital interactions. These results provide new insights into the electronic nature of porphyrin-ligand interactions.