

## **Department of Chemistry**



## 9:45 a.m. Thursday, December 5 • 331 Smith Hall



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## Electronic Spectra and Electronic Structure of Transition Metal Molecules

Research interests: understanding the chemical bonding and electronic structure in metallic and semiconductor systems by detailed spectroscopic investigations.

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## Abstract

The transition metals are known for their chemical diversity, being capable of exhibiting a wide variety of oxidation states and modes of chemical bonding. The ability to engage in a wide range of chemical bonding modes makes the transition metals excellent agents of catalysis while simultaneously making their theoretical description quite challenging. The computational challenges are particularly severe in the diatomic transition metals, which can exhibit high spin states characterized by magnetic interactions between atoms, low spin states with high-order multiple bonds between atoms, and everything in between. In this lecture, I will describe the electronic structure as revealed through optical spectroscopy, progressing from the coinage metal dimers (Cu<sub>2</sub>, Ag<sub>2</sub>, Au<sub>2</sub>), to systems in which one or both of the d<sup>10</sup> cores are opened (NiCu, Ni<sub>2</sub>, Pt<sub>2</sub>), and eventually to systems with high-order multiple bonds (Cr<sub>2</sub>, CrMo, Mo<sub>2</sub>, VCr, NbCr, VMo, NbMo, TiFe, and ZrFe). Along the way, the relevance of charge-transfer states and ligand field theory to these peculiar molecules will be examined.