



# CHEMISTRY SEMINAR 291

## **Correlated, One-Electron Theories of Chemical Bonding and Spectra: Applications to Exotic Anions**

Date: 2/28/20

Time: **3:00—4:20 PM**

Location: **COB1 267**

**Joseph Vincent Ortiz**

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### Abstract

Ab initio molecular electronic structure theory aims at the prediction of observables and at revealing qualitative relationships between them. Molecular-orbital or valence-bond methods often succeed at one of these aims while failing at the other. The dilemma of accuracy versus interpretability may be resolved with electron propagator theory. Dyson orbitals and electron binding energies obtained efficiently with the Dyson equation provide a complete, one-electron picture of chemical bonding that is experimentally testable.

Applications to super-halogens, correlation-bound anionic clusters, solvated-electron precursors and double Rydberg anions provide examples of the power of electron propagator theory in the discovery and interpretation of novel patterns of molecular electronic structure.

### About the Speaker

**J. V. Ortiz** was born in Bethpage, New York in 1956 and attended public schools in Plainview, New York until 1973. After obtaining a B.S. in Chemistry with High Honors at the University of Florida in 1976, he began graduate work in the Quantum Theory Project of the same university and completed his dissertation in 1981 under the supervision of Yngve Öhrn, earning a Ph.D. in Chemistry with a certificate in Chemical Physics. After two years as a postdoctoral fellow at Harvard University with William Lipscomb and at Cornell University with Roald Hoffman, he spent thirteen years at the University of New Mexico. In December, 1996, he joined the Chemistry Department of Kansas State University and was named a University Distinguished Professor in April, 2004. He became the first Ruth W. Molette Professor of Chemistry and Biochemistry at Auburn University in August, 2006 and simultaneously began serving as Chairman of the Department of Chemistry and Biochemistry. His second, four-year term ended in August, 2014.

