JMU Chemistry and Biochemistry Seminar
Friday, October 16, 2015
3:35pm in ISAT 159

Dyson Orbitals and New Kinds of Chemical Bonding

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Electron propagator theory enables ab initio calculation of electron binding energies and associated Dyson orbitals without solving for many-electron wave-functions and provides an exact generalization of molecular orbital concepts. Pictorial interpretations of accurate calculations enable the prediction of novel patterns of electronic structure such as delocalized electrons in aqueous fluoride solutions, fullerides in diffuse, excited states and double Rydberg anions.