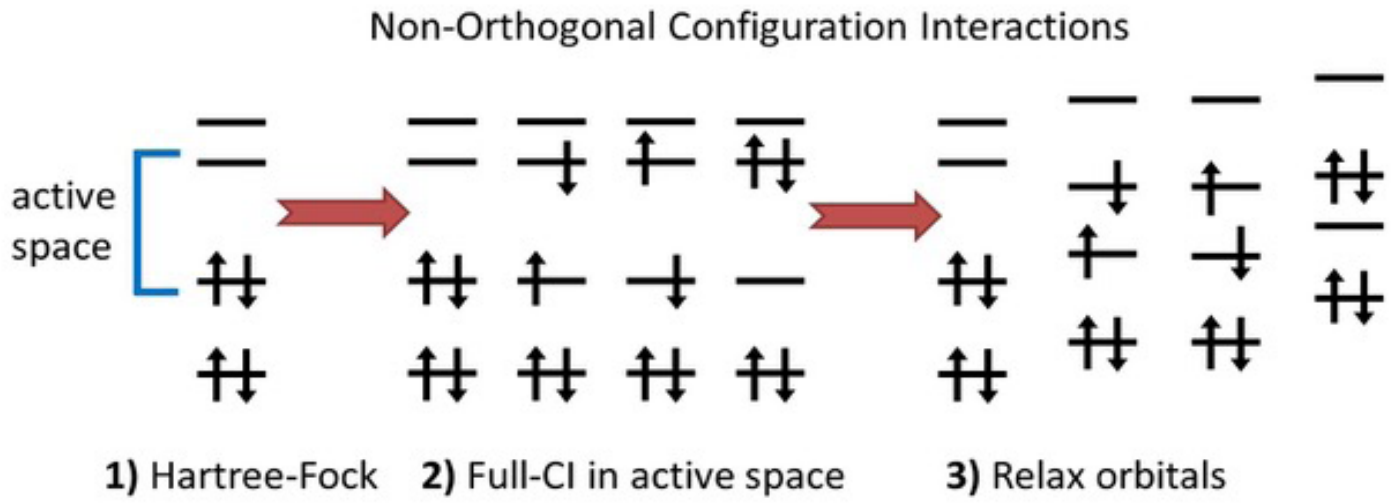
New Excited State Multi-Reference Method with Application to Singlet-Triplet Gaps and Weakly Bonded Systems



Science & Mathematics Colloquium Series

Presentation by Shane Yost

Postdoctoral Fellow, University of California, Berkeley

Mon., March 20, 2017, 3 pm

Cooley Ballroom, Student Union
ASU Polytechnic campus

Most advanced electronic structure methods for strongly correlated systems use an active space approach, the most common of which is the complete active space self-consistent field theory (CASSCF). The issue with most active space approaches is that a large active space is required to obtain accurate results for the ground and excited states.

Shane Yost will present a new multi-reference excited state method that uses a non-orthogonal approach to the wave functions, called NOCI-MP2. The use of non-orthogonal molecular orbitals allows one to use a much smaller active space in large systems. NOCI-MP2 is applied to a number of molecular systems with small singlet-triplet gaps, the dissociation of di-diamantane ethane, and other weakly bonded systems.

Shane Yost earned a BS from the University of California, Santa Barbara, in chemistry and biochemistry. He then went on to complete a PhD in physical chemistry at MIT, working for Professor Troy Van Voorhis. While at MIT he studied different aspects of organic photovoltaic devices, including exciton absorption, transport, singlet fission, and charge separation.

Dr. Yost is now a postdoctoral fellow at the University of California, Berkeley, working with Professor Martin Head-Gordon. His current work focuses on the development of new multi-reference electronic structure methods for ground and excited states.

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