LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

Fall Seminar Series

3:30pm - 4:30pm, Wednesday, December 5, 2012

Tulane University

Lindy Boggs, Room 242

Symmetry Breaking and Restoration

by

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Abstract: I will present our recent results on the calculation of symmetry-projected wave functions [1,2] for electronic structure theory. For Hartree-Fock and spin projection, this is a 50-year old problem in quantum chemistry, going all the way back to Löwdin and his "extended HF" theory. For Hartree-Fock-Bogoliubov and number projection, our approach offers new perspectives on Antisymmetrized Geminal Power (AGP) wavefunctions that were the focus of much attention in the 1980s. In our work, all molecular symmetries (electron number, spin S^2 and S_z , point group, and complex conjugation) are deliberately broken and restored in a self-consistent variation-after-projection approach. The resulting method yields a comprehensive black-box treatment of static correlation with one-electron (mean-field) computational cost. The ensuing wave function is of high quality multireference character competitive with exact diagonalization. The method can also be applied to calculate excited states and spectral functions [3]. The curse of the thermodynamic limit and the quest for a low-cost treatment of residual correlations will also be addressed.

Biography: Gustavo E. Scuseria is the Robert Alonzo Welch Professor of Chemistry and Professor of Physics & Astronomy at Rice University in Houston, Texas. He joined the faculty at Rice in 1989. Professor Scuseria is a US citizen born in Argentina. He received his Ph. D. in Physics from the University of Buenos Aires in 1983. After moving to UC Berkeley in 1985, his interest in electronic structure theory steered him to the quantum chemistry field. Over the years, he has straddled between chemistry and physics, working in diverse areas ranging from coupled cluster to density functional theories and with applications to both molecules and solids including actinide oxides and carbon nanostructures.