

Quantum Chemistry for Strong Correlation

Gustavo E. Scuseria

Department of Chemistry, Department of Physics & Astronomy, Department of Materials Science & Nano Engineering, Rice University, Houston, Texas, USA
guscus@rice.edu

Schrodinger's equation has been known for more than 90 years, yet many pressing questions in electronic structure theory remain unanswered. Quantum Chemistry is a successful field because for weakly correlated problems, we can get accurate answers at reasonably low polynomial computational cost instead of the combinatorial expense of brute force approaches. Despite many advances, however, the so-called strong correlation problem, where the chemist's molecular orbital picture breaks down, remains quite open, particularly for large molecules and solids. This lecture will address challenges and progress on the treatment of strong correlation, and its connection with quantum symmetries and degeneracy. Methods recently developed in our research group for strong correlation will be discussed.