MARVEL

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

# NCCR MARVEL Distinguished Lecture

# The strong correlation problem: A quantum chemistry perspective

*Prof. Gustavo E. Scuseria,*
*Department of Chemistry, Department of Physics and Astronomy,*
*Department of Materials Science and NanoEngineering*
*Rice University, Houston, USA*

Tuesday 13th January, 16:15, Room MXF-1

**Abstract:** Computational quantum chemistry is a very successful field. However, 89 years after Schrodinger's equation, strongly correlated systems remain outside the realm of accurate calculations. The reigning wavefunction paradigm, coupled cluster (CC) theory with single and double excitations, accurately describes weak electron correlation but is known to fail in cases of strong correlation. The same is true for density functional approximations. This talk will address recent efforts in our research group to deal with strongly correlated systems, including bulk systems, using first principles wavefunction methods. Our models make extensive use of similarity transformed Hamiltonians and the concept of pairing, but they do so utilizing two different bases: one is defined by the traditional reference determinant and the other one by the correlator themselves. Using those models as impurity solvers, we can study bulk systems using quantum embedding theories. This talk will discuss how quantum chemistry inspired tools can address the challenge of strongly correlated materials.

[1] Seniority-based coupled cluster theory, T. M. Henderson, I. W. Bulik, T. Stein, and G. E. Scuseria, *J. Chem. Phys.*, http://arxiv.org/abs/1410.6529
[2] Lie-algebraic similarity transformed Hamiltonians for lattice model systems, J. Wahlen-Strothman, C. A. Jimenez-Hoyos, T. M. Henderson, and G. E. Scuseria, *Phys. Rev. B.*, http://arxiv.org/abs/1409.2203
[3] Electron correlation in solids via density embedding theory, I. W. Bulik, W. Chen, and G. E. Scuseria, *J. Chem. Phys*

FNSNF
Swiss National Science Foundation The National Centres of Competence in Research (NCCR) are a research instrument of the Swiss National Science Foundation.