SYLLABUS FOR CHM 7485. Fall 2013.

"Special Topics in Theory of Atomic and Molecular Structure"

Instructor: Dr. Bartlett.

TEXT: Not mandatory but copies should be available for all.

Isaiah Shavitt and R. J Bartlett,

"Many-Body Methods in Chemistry and Physics: MBPT and Coupled-cluster Theory"
Cambridge Molecular Science

I. Why coupled-cluster theory?
   Extensivity. Power of exponential wavefunction.
II. Systematic development of CC tools.
   Second-quantization
   Normal Ordered Operators
   Wick's Theorem-Contractions
III. Coupled-cluster doubles Eqns.
   Algebraic Derivation
   Diagrammatic derivation

IV. CCSD Eqns.
V. CCSDT Eqns.
   CCSD(T)
VI. Analytic Gradients and Properties
VII. Equation-of Motion CC Method for Excited States
VIII. Multi-reference Approaches.