SYLLABUS FOR CHM 7485. R. J. Bartlett, Tuesday, Thursday, 10:30 to noon, New QTP Conference room, Leigh, 240 E.

TEXT: Not mandatory but copies should be available.

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
   Connections with Perturbation Theory
IV. CCSD Eqns.
V. Density Matrices
VI. CCSDT Eqns.
   CCSD(T)
   CCSDTQ_f
   CCSDT(Q)
VII. Distinguished Cluster Approximations
VIII. Analytic Gradients and Properties
IX. Equation-of Motion CC Method for Excited States
   IP/EA-EOM-CC
   EE-EOM-CC
X. STEOM-CC