

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
- XI. Hilbert Space-Multi-reference Approach.