

## SYLLABUS FOR CHM 7485.

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.

