

The following books are highly recommended for supplemental reading:

[Electronic structure theory](#)

Modern Quantum Chemistry, A. Szabo and N.S. Ostlund (MacMillan, but now available through Dover)

Exploring Chemistry with Electronic Structure Methods, J. B. Foresman and Á. Frisch (Gaussian, Inc.)

[Monte Carlo and MD simulations](#)

Computer Simulation of Liquids, M. P. Allen and D. J. Tildesley (Oxford Univ. Press)

Understanding Molecular Simulation, D. Frenken and B. Smit (Academic Press)

[MD and MC simulations as well as electronic structure theory](#)

Introduction to Computational Chemistry, F. Jensen (John Wiley & Sons)

Web links with useful information (to be added):