Reading List

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1 Electronic Structure

1) Modern Quantum Chemistry - Introduction to Advanced Electronic Structure Theory
Attila Szabo and Neil S. Ostlund.
Chapters 1, 2, 3, 4 and 6.

2) DFT in a Nutshell
Kieron Burke and Lucas O. Wagner
International Journal of Quantum Chemistry 2013, 113, 96-101

3) Importance of short-range versus long-range Hartree-Fock exchange for the performance of hybrid density functionals
Oleg A. Vydrov, Jochen Heyd, Aliaksandr V. Krukau, and Gustavo E. Scuseria
Journal of Chemical Physics 2006, 125, 074106

2 Molecular Dynamics

1) Background notes written for students in the Welborn group.

2) Molecular Dynamics Simulations and Drug Discovery
Jacob D. Durrant and J. Andrew McCammon
BioMed Central Biology 2011, 9, 71

3) Polarizable Force Fields for Biomolecular Simulations: Recent Advances and Applications
Zhifeng Jing et al.
Annual Review of Biophysics 2019, 48, 371-394

4) The Diabatic Picture ofElectron Transfer, ReactionBarriers, and MolecularDynamics
Troy Van Voorhis et al.
Annual Review of Physical Chemistry 2010, 61, 149–170

5) Molecular dynamics with electronic transitions
John C. Tully
Journal of Chemical Physics 1990, 93, 1061

3 Statistical Mechanics

1) Textbook "Statistical Mechanics"
Donald A. McQuarrie

2) Textbook "Understanding Molecular Simulation: From Algorithms to Applications"
Berend Smit and Daan Frenkel
Chapters 2,4,6 and 7