This is an attempt to start collecting the ideas for each chapter and what we may need. It serves as an organization of ideas mostly. It is also a good way for me to relearn to use TeX and the software again. I can use the practice.I assume that best way to proceed will to make each chapter a different file and work on them separately. In fact on the publisher's web page of instructions they want each chapter as aseparate file it looks like. We could divide them to do the first drafts. One start would be: Tony - 4,5; Henry - 2,3. We should talka bit more about 1, 6, and 7. The sections are based on what was inthe proposal and I expect they will change a lot as it goes. It seems they like LaTex and take the results as PDF files. There is a template we can get after they make an agreement with us.

Chapter 1

Why Bigger is Better

1.1 The role of modern computer architecture

1.2 The convergence of theory and experiment: the mesoscopic world

Experiments are probing smaller but still a need for larger and larger theory to actually match.

1.3 Quantum effects in biology

Need a discussion of motivation. That computational biochemistry islargely non-electron and empirical. Can do better than that,particularly if interest in reactions not just structures.

1.4 Qualitative versus Quantitative Descriptions

Chapter 2

A Brief Review of Quantum Chemistry

2.1 Hartree-Fock Theory

2.1.1 Basis Set Discussion

2.1.2 Inclusion of Correlation

2.2 Density Functional Theory

2.3 Semiempirical Quantum Chemistry

Short discussion of popular schemes Mozeyme

2.4 Approaches to Large Molecules

2.4.1 Fragment-based Methods

2.4.2 Linear-Scaling Methods

2.4.3 The ONIOM method

2.4.4 Local Orbitals versus Canonical Orbitals

2.4.5 Plane Wave Approximations

2.4.6 NBO Analysis

2.5 Something about Molecular Mechanics?

Chapter 3

A Primer for Condensed Matter Physics

3.1 Solvent Effects in Electronic Structure Calculations

3.2 Density of States

3.3 The Kronig-Penny Model

3.4 Semiconductors

3.5 The Tight-Binding Model

3.6 Band Structure

Chapter 4

Electronic Structure for Nucleic Acid Systems

First part is background on nature of nucleic acid structures and into to questions and previous calculations.Need List of calculations done that will be included and discussed.

4.1 Start Small: Early Studies of DNA Bases

4.2 Large-scale Calculations of Electronic Structure

4.2.1 Convergence Issues

4.2.2 Linear Scaling Approximations

4.2.3 Fragment Based Treatments

4.3 Case Study: Ecteinascidin 743

4.3.1 How Big is Big Enough

4.3.2 It's all about the orbitals

Chapter 5

Electronic Structure for Amino Acid Systems

5.1 Why Proteins Differ from DNA: An Electronic Structure Perspective

5.1.1 Nitrogen as an insulator?

5.2 Taking a Big Bite

5.3 Convergence Characteristics

5.4 Comparison of Linear Scaling and FMO Methods

5.5 Case Study: Dihydopteroate Synthase

5.5.1 When do you really need all the protein

5.5.2 Orbital Steering and Quantum Chemistry

Need List of calculations done that will be included and discussed.

Chapter 6

Electronic Structure for Semiconductor Systems

6.1 Periodic Treatments

6.2 Can we get Band Stricture Directly?

6.3 What do we lose in the approximations

6.4 Case Study: ?????

Options:SiO2 systemsanother system

Chapter 7

General Considerations

7.1 Asking the Right Questions

7.2 What Do We Lose With Approximate Methods

7.3 Is Bigger Always Better?

7.4 How Large Can We Go?

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[2] W. J. Stevens, M. Krauss, H. Basch, and P. G. Jasien, *Can. J. Chem.* **70**, 612 (1992); T. R. Cundari and W. J. Stevens, *J. Chem. Phys.* **98**, 5555 (1993).