## Physics 685 – Electronic Structure

Please read Martin, Electronic Structure, Chapter 2, section 10. Please read Martin, Chapter 3.1, 3.2, 3.3 "a" and Griffiths, Quantum Mechanics, Chap. 7, especially 7.3 on the $H^+$ ion.

1. What does the book have to say about the following issues in 2.10?

   (a) What is the fundamental band gap? Is the fundamental band gap of a semiconductor properly considered a ground state property or excited state property of the system? Or possibly neither?

   (b) In what sense is the difficulty in obtaining accurate calculations of the band-gap in DFT a *technical* issue or a *fundamental* one? (Do we need to go beyond DFT or just improve approximate DFT's?)

2. Problem 7.x, Griffiths – the antibonding state of the Hydrogen ion.

3. Try problem 3.3, Martin – Forces. Please note error in equation 3.18 – the last term is already part of the $\partial H/\partial R$ term preceding it.