## Updated Schedule (as for 03/25/20)

Table 2: The list of lectures and respective chapters in McQuarrie. The homework due dates are shown

in bold.

| #   | Class/HW due | Day          | Lecture  | Chapters                             |
|-----|--------------|--------------|--|--------------------------------------|
| XXX | 03-27-20     | F            | Recalibration Period for Education Equity          | _                                    |
| L13 | 03-31-20     | ${ m T}$     | Introduction to Approximation Methods <sup>a</sup> | CH7                                  |
| L14 | 04-03-20     | $\mathbf{F}$ | Multielectron Atoms                                | CH 8                                 |
| В   | 04-07-20     | Τ            | No Class   |                                      |
| В   | 04-10-20     | $\mathbf{F}$ | No Class   |                                      |
| L15 | 04-14-20     | Τ            | Multielectron Atoms - Terms                        | CH 8                                 |
| L16 | 04-17-20     | $\mathbf{F}$ | Diatomic Molecules I                               | CH 9                                 |
| L17 | 04-21-20     | ${ m T}$     | Diatomic Molecules II                              | CH 9                                 |
| L18 | 04 - 24 - 20 | $\mathbf{F}$ | Polyatomic Molecules I - Hybrid Orbitals           | CH 10                                |
| L19 | 04-28-20     | ${ m T}$     | Polyatomic Molecules II - Hückel Model             | CH 10                                |
| L20 | 05-01-20     | F            | Molecular Spectroscopy - Introduction              | CH 13                                |
| L21 | 05-05-20     | ${ m T}$     | Advanced Molecular Spectroscopy                    | PowerPoint                           |
| L22 | 05-08-20     | $\mathbf{F}$ | Comutational Chemistry & Molecular Spectroscopy I  | $Assignment^b$                       |
| L23 | 05-12-20     | ${ m T}$     | Comutational Chemistry & Molecular Spectroscopy II | Assignment <sup><math>b</math></sup> |
| В   | 05-15-20     | $\mathbf{F}$ | Reading Day  |                                      |
| FIN | 05-19-20     | ${ m T}$     | Final Exam (Parts 3 and 4, 11.30 - 1.30 pm)        |                                      |

<sup>&</sup>lt;sup>a</sup> There is no class on this day, however I will still post the lecture in the morning. I will hold Office hours on Thu to answer questions regarding the lecture.

- 1. Force Fields and Molecular Dynamics Simulations
- 2. Hartree-Fock and Electron Correlation
- 3. Density-Functional Theory (1998 Nobel Prize in Chemistry)
- 4. QM/MM techniques for large biomolecules (2013 Nobel Prize in Chemistry)
- 5. Gas-phase spectroscopy of biomolecules
- 6. Spectroscopic methods in several kelvins
- 7. Raman and other types of vibrational (non-IR) spectroscopy
- 8. Specroscopic methods in astrophysics and astrochemistry

<sup>&</sup>lt;sup>b</sup> Exemplary topics for the assignment: