**Lucy Whalley Corrections list**

**Front matter**

p.8 Ambiguity over who prepared Fig.2.3

p.17 If need to give values should use higher precision

**Chapter 1**

p.27 Refs needed for equations 1.5-1.9

p.30 A more careful description of mobility should be given including discussion of the Drude model

**Chapter 3**

Section 3.2 on DFT lacks sufficient detail on most of the methods and theoretical concepts that underpin this work in this thesis and needs to be substantially rewritten after the candidate and properly refreshed her understanding. This includes description of the many electron schrodinger equation, Hartree-Fock and exchange, the Kohn-Sham equations, GGA, the HSE functional including range dependence, discussion of Bloch functions and reciprocal space and the PAW method.

p.49 Eq. 3.2 should show that the many-body wavefunction is a function of the coordinates of all N electrons not just of them.

p.50 The right equation in Fig. 3.1 uses total energy E rather than single particle energy e\_i

p.53 The discussion of Meta-GGA is too brief to be useful but may be omitted entirely since it is not used.

p.61 Misleading statement on growth conditions

**Chapter 4**

p.71 Fig. 4.1 central panel is confusing. The dashed curves appear to have nothing to do with the second derivative.

p.74 Eq. 4.11 is dimensionally inconsistent and does not specify at which point the second derivative is evaluated. Assume it is point i I believe the equation has errors in both the numerator and denominator. This equation was not derived (taken from literature) but there is no citation. It should be confirmed this equation is not used in the code.

p.74 Also need to give expression for evaluation of dE/dk

p.81 Size of symbols in Fig. 4.6 and 4.7 very large and scale makes it difficult to see trend

**Chapter 5**

p.89 Need to explain where Eq. 5.1 comes from.

p.89 Eq. 5.2 seems inconsistent as **k** does not appear.

p.90 ‘long carrier lengths’ – meaning unclear

p.91 Include ref for displacement step size selected.

p.95 Issue with x-axis symbol format in Fig. 5.3 and 5.5

p.97 More detailed discussion of the idea of an excited polaron

p.98 Define valence and conduction band deformation potential

**Chapter 6**

p.104 Explain why this particular supercell expansion

p.105 Missing delta in Eq. 6.1

p.106 Where does eq.6.2 come from?

p.108 More details of dielectric embedding approach needed.

p.117 Some statements about valence when actually mean conduction

p.119 Hole capture -> hole emission

**References**

Several cases of inconsistent journal name abbreviation which should be corrected (note not all identified in annotated pdf).