SUMMARY OF WEEK 1

⇒ microscopic phenomena cannot be described by classical physics

– partcile-wave dualism, discrete energies (spectra), photoelectric effect .....

– Schrödinger equation is the suitable description

→ energy levels (eigenvalues), ZPE, 'wave'functions (interferences)

quantum mechanics → classical mechanics

when m and T large (for 'free' systems ie. ZPE << $k_{\mathrm{B}}T$)

⇒ In chemistry (ie at energies $E = k_{\mathrm{B}}T$ with $T \approx 100...1000$ K)

Born-Oppenheimer approximation : treat electrons and nuclei separately

⇒ Electronic Schrödinger Eq. ("Quantum chemistry" (ab-initio. DFT .....))

→ compute electronic ground state energies and determine PES

⇒ fitting

(what does a "fit" mean, inter- and extrapolation, overfitting)

⇒ PES

intra- and intermolecular PESs, minima, transition points ...

→ find suitable ansatz functions (models) to represent a PES

eg. LJ model, (more LATER)

⇒ Nuclei: mostly classical mechanics (m and T large enough)

(except molecular vibrations because ZPE too high (Δx too small,

see particle in box or harm.oscil.) (more LATER)

Week 2

⇒ How to deal with many particle (molecule) systems (condensed phases, liquids, solids ...)

LJ: Lennard-Jones

PES: Potential Energy Surface

ZPE: Zero Point Energy