A1) ΔU and ΔG are state functions

A2) verlet velocity integer is used in monte Carlo Simulation.

A3) [illegible]

B1) In force field ther are Non-covalent interactions, chose two and explain them in detail.

B2) Explain the difference between ab initio force field and PES.

B3) Describe the proeties of molecular dynamics.

A1) The First Principle of thermodynamics provides a criterion to determine the spontaneity of a chemical reaction or transformation.

A2) Stacking interactions are peculiar of hydrogen atoms covalently bonded to electronegative atoms.

A3) Euler's integrator is very accurate and preserves very well the total energy during the simulation.

B1) Describe the possible types of dispetion interaction

B2) Elaborate on the different ways the solvent can be taken into account in computational simulations

B3) Describe in details two examples of trade-off between computational cost and accuracy.

A1) TO see if a system is spontaneous, a combination of ΔS and ΔH is enough

A2) explicit is computationally cheaper than implicit solvation.

A3) Repulsion force which is defined by $1/r^{12}$ is based on newtons law of motion.

B1) What covalent interaction is used in Forcefield. Describe all.

B2) What is the role of thermostat. What are different types and explain all.

B3) with molecular dynamics you can study the time-dependent properties of a system. What are these properties and explain all.