In class work

1. **Para- and Ortho-hydrogen.** Para and orthohydrogen are spin isomers of the hydrogen molecule \( H_2 \). First consider the states of the electrons that contribute to bonding, what bonding orbital do they occupy?

Now consider the nuclei—there are two protons. Because protons have spin-\( \frac{1}{2} \), we need the nuclei to also form an overall antisymmetric total wavefunction. Orthohydrogen refers to the triplet state configuration for the spin wave functions: what are these? Given that the triplet spin state corresponds to a symmetric linear combination, the *rotational* state must be anti-symmetric. What values of \( \ell \) do these correspond to?

Parahydrogen corresponds to the spin singlet state (what is this?), which is anti-symmetric, so requires the symmetric rotational states. Given that \( H_2 \) has a bond length of (74 pm), what is the energy difference between the lowest energy state for parahydrogen versus orthohydrogen? (Express your answer in Kelvin-\( k_B \))

Using what we learned from statistical mechanics, write an expression for the ratio of orthohydrogen to parahydrogen molecules at temperature \( T \). Don’t forget about the degeneracy of the spin and rotational states.
2. Consider the cases of hydrogen bonding with fluorine and sodium bonding with fluorine.
   a) In each case how close must the atoms approach to reach the “break even” point where the 
electrostatic potential energy compensates for the ionization energy and electron affinity. The 
ionization energy of hydrogen is 13.6 eV (which you should already know), for Sodium it is 
5.139 eV and the electron affinity for fluorine is 3.40 eV.
   b) One of these molecules is considered to have an ionic bond and the other is considered to 
have a covalent bond, which is which and why?

3. The Lennard Jones potential is,
\[ V_{LJ}(r) = 4\epsilon \left[ (\sigma/r)^{12} - (\sigma/r)^6 \right] \]  
(1)
Here, \( \epsilon \) is a parameter that gives the strength of the potential. Determine the distance \( r_{min} \)
that minimizes the potential energy.