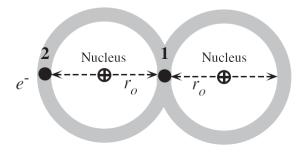
HW #3

- 1. **(Kasap 1.3) The covalent bond** Consider the H_2 molecule in a simple way as two touching H atoms, as depicted in the figure. Does this arrangement have a lower energy than two separated H atoms? Suppose that electrons totally correlate their motions so that they move to avoid each other as in the snapshot in the figure. The radius r_0 of the hydrogen atom is 0.0529 nm. The electrostatic potential energy of two charges Q_1 and Q_2 separated by a distance r is given by $Q_1Q_2/(4\pi\epsilon_0 r)$. Using the virial theorem consider the following:
 - a. Calculate the total electrostatic potential energy PE of all the charges when they are arranged as shown in the figure. In evaluating the PE of the whole collection of charges you must consider all pairs of charges and, at the same time, avoid double counting of interactions between the same pair of charges. The total PE is the sum of the following: electron 1 interacting with the proton at a distance r_0 on the left, proton at r_0 on the right, and electron 2 at a distance $2r_0$, plus electron 2 interacting with a proton at r_0 and another proton at $3r_0$, plus two protons, separated by $2r_0$, interacting with each other. Is this configuration energetically favorable?
 - b. Given that in the isolated H atom the PE is 2 x (-13.6 eV), calculate the change in PE in going from two isolated H atoms to the H₂ molecule. Using the virial theorem, find the change in the total energy and hence the covalent bond energy. How does this compare with the experimental value of 4.51 eV?



Hydrogen Hydrogen