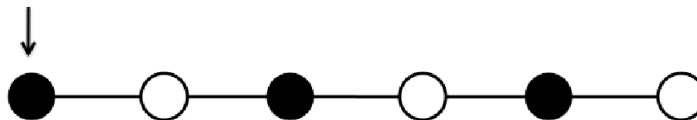


Consider the finite linear molecule presented in the figure, made of alternating H (open circles) and Li (black circles) atoms. This can be described by a nearest neighbor tight-binding model using the H  $1s$  and Li  $2s$  atomic orbital as basis functions. Define the hopping parameter as  $t$  and the on-site energies for H and Li respectively as  $\epsilon_{\text{H}}$  and  $\epsilon_{\text{Li}}$ .



1. Calculate the energy spectrum of such a molecule when the parameters of the model are  $t = -2$  eV,  $\epsilon_{\text{H}} = -1$  eV and  $\epsilon_{\text{Li}} = 1$  eV (write explicitly the numerical values of the eigenvalues).
2. Draw schematically the wave-function for the lowest eigenvalue (the explicit calculation of the wave-function is not required).
3. What is the quantum mechanical probability to find an electron on the left-most Li atom of the molecule (the one indicated by the arrow), when the electron occupies the second lowest of the eigenvalues ?
4. Calculate the total electronic energy when the molecule contains 3 electrons and when the molecule contains 6 electrons.