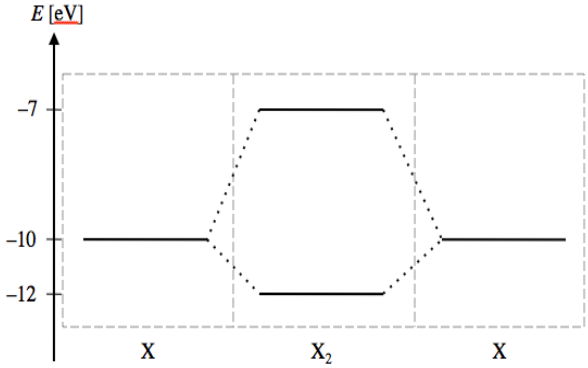
27. Reaction enthalpies from correlation diagrams

When two atoms bond, they form molecular orbitals. Some of these orbitals are lower in energy than the initial atomic orbitals, while some are higher in energy. The bond enthalpy is the amount of energy required to break apart a bond. For diatomic molecular bonding (bonding between two identical atoms), correlation diagrams are an easy way to calculate this change in energy.

$$\text{Reaction enthalpy} = \text{change in energy for a reaction} = E_f - E_i \qquad (1)$$

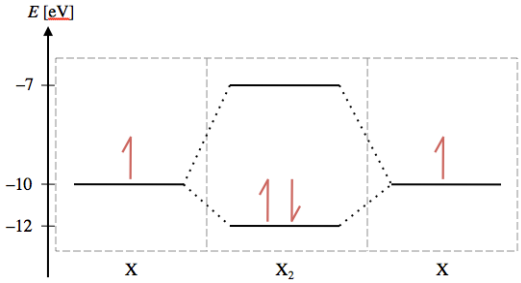
To see how the electron energy changes when molecules are formed, broken apart, or ionized, a fictitious element "X" will be used. The correlation diagram below shows the atomic and molecular orbitals for element "X" and molecule "X_2". For the element X, the only electron involved in bonding has an energy of -10eV (as seen in the diagram).



Worked Example

1) Calculate the energy change for the formation of an X_2 molecule from two X atoms:

$X + X \rightarrow X_2$



The initial energy is the energy of the electrons in atomic orbitals: $E_i = 2\ (-10\text{eV}) = -20\text{eV}$

The final energy is the energy of the electrons in molecular orbitals: $E_f = 2\ (-12\text{eV}) = -24\text{eV}$

$$\begin{aligned}\Delta E &= E_f - E_i \\ &= (-24\text{eV}) - (-20\text{eV}) \\ &= -4\text{eV}\end{aligned}$$

To calculate the energy change for the formation of X_2, the initial and final energies must first be calculated. In this example, each X atom has an electron in a –10eV orbital. Therefore the initial energy is twice this energy. Similarly, the final energy is twice the energy of the molecular orbital, –12eV, because there are two electrons in this orbital. The energy change of reaction shows that creating the molecule X_2 from X + X releases 4eV of energy (as we expect).

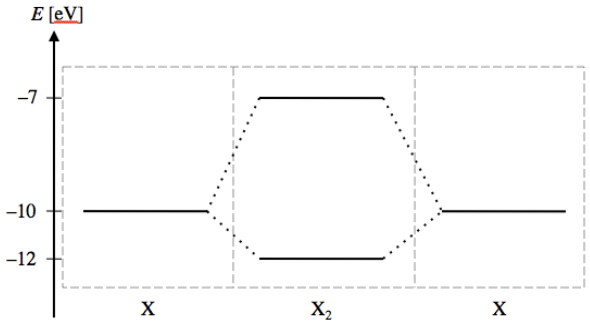
2) Calculate the energy required to cleave the X_2 bond (bond enthalpy of X_2).

$X_2 \rightarrow X + X$

$E_i =$

$E_f =$

$\Delta E = \Delta_b H =$



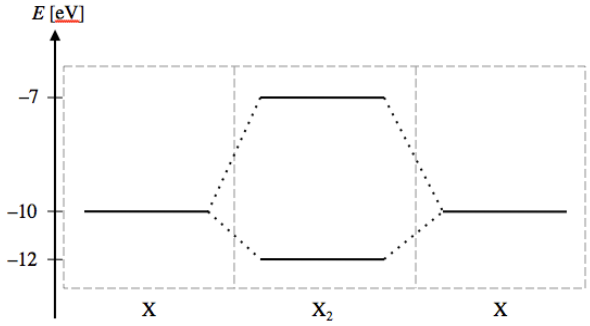
3) Following the same approach, calculate the ionization energy of an X_2 molecule:

$X_2 \rightarrow X_2^+$

$E_i =$

$E_f =$

$\Delta E =$



4) Following the same approach, calculate the energy of reaction for the formation of an X_2 molecule from two ions:

$X^+ + X^- \rightarrow X_2$

$E_i =$

$E_f =$

$\Delta E =$