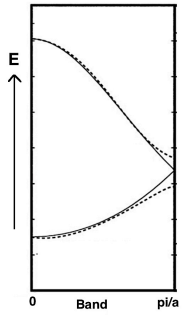
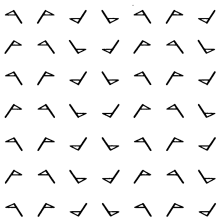
I. Calculate $\Delta G^{\ddagger}$ at 298 K for the reaction 2N + H ----> N_2 + H.
Consider $E_a = 5.4\ k\ J\ mol^{-1}$ and $\Delta S^{\ddagger} = 32.6\ J\ K^{-1} mol^{-1}$

II. For the band dispersion given below, sketch schematic density of states (DOS).

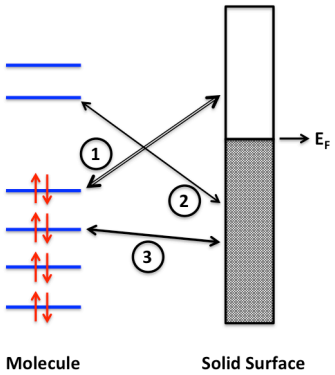


III. From the schematic representation of the periodic two-dimensional tiling pattern that is shown below, calculate the total number of basis required to construct a unit cell. Mark the unit cell that was found.



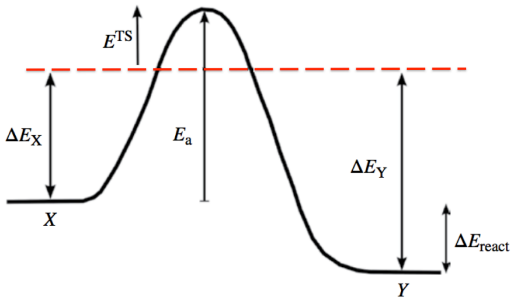
IV. In the spirit of one electron picture and frontier molecular orbital energy levels diagram, the interaction of a molecule (for example N_2) with iron metal surface has been depicted below. Each one of these interactions indicated involve in charge transfer are labeled with numeric digits. Explain the cases in which interactions

(a) The molecule is donor or acceptor and like-wise the surface is donor or acceptor.
(b) Which interactions are repulsive and attractive? Offer schematic energy level diagrams indicating the features of repulsive and attractive interactions for diagram shown below.



V. Graphically illustrate the Bell–Evans–Polanyi (BEP) principle for a series of similar chemical reactions in both endothermic and exothermic cases. For illustrating the evolution of enthalpies consider at-least 5 reaction profiles. The schematic graph must be appropriately labeled with all the components depicting the BEP.

VI. A schematic potential energy surface (PES) is shown below represents a transition between two minima X and Y. The dashed (red color) line defines the energy reference. Let's say the E^{TS} be a set of energies describing the energy needed to move between the two minima on the PES for a set of different catalysts. For this, construct a functional form that describes the BEP relation.



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