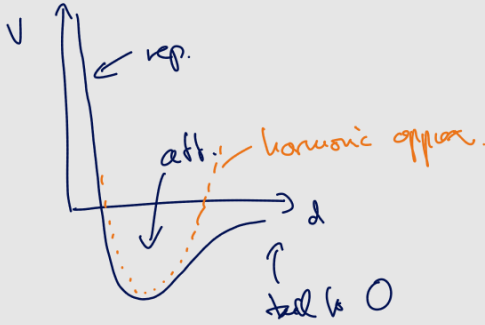


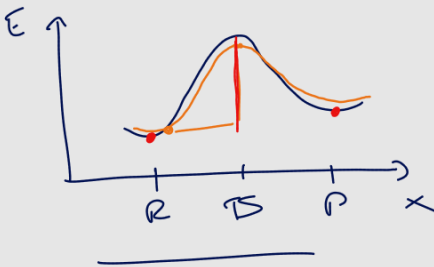
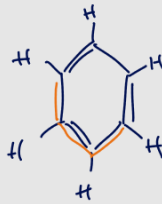
$$\frac{\partial E}{\partial x} = 0 \quad \left[\frac{\partial^2 E}{\partial x^2} \right]$$

$$f(x) = ax^2$$



Bonds: Morse

Clusters: Lennard Jones



- all everything

- critical points only

$$(R, P) \rightarrow E_R, E_P, E_a$$

$$\frac{1}{2} a (b - b_0)^2$$

$$\frac{1}{2} \cdot \left(\begin{matrix} | \\ - \\ \cdot \end{matrix} \right)^2$$

$$\downarrow$$

$$\begin{matrix} | \\ \vdots \\ | \end{matrix} \rightarrow |$$

$$\frac{1}{2} \cdot |^2 \Rightarrow \cdot | \rightarrow \vdots | \rightarrow |$$

• scalar

| array



Ureg-Droelley

