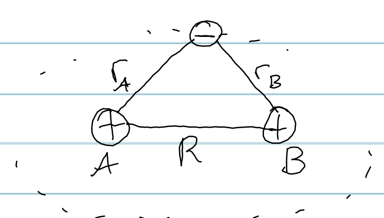
Vorlesung 13.12.2013

Nachtrag zu gestern: Copernicium → ~~Cm~~ Cn!

OZ	Chem. Symbol	$\tau_{1/2}$
107	Bh	17 s
108	Hs	25 s
109	Mt	42 ms
110	Ds	56 ms
111	Rg	6,4 ms
112	Cn	0,6 ms

6 Moleküle und chemische Bindung

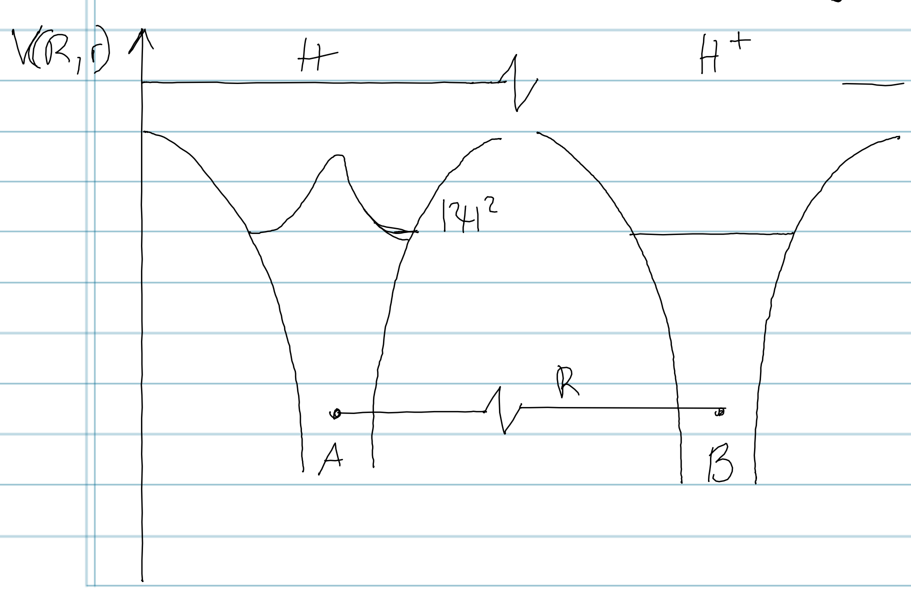
Wasserstoffmolekül-Ion H_2^+

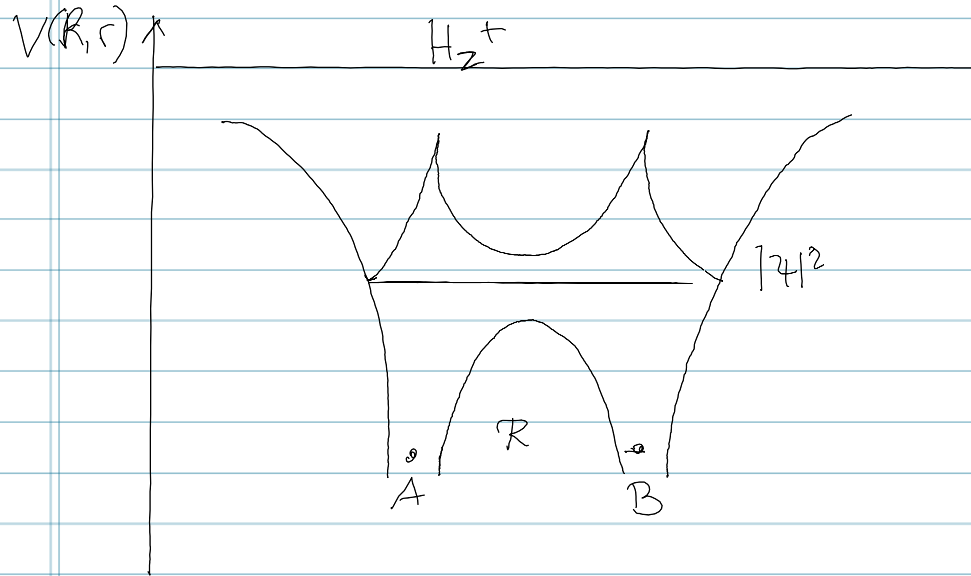


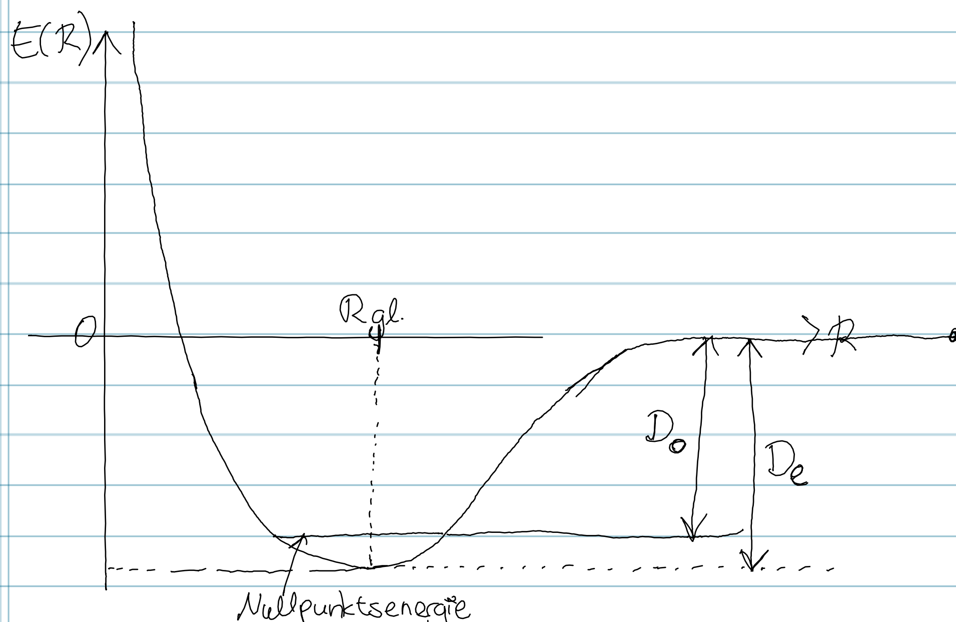
$R = 1{,}06$ Å

Bindungsenergie: 2,79 eV

Pot. Energie: $V(R,r) = -\frac{e^2}{r_A} - \frac{e^2}{r_B} + \frac{e^2}{R}$



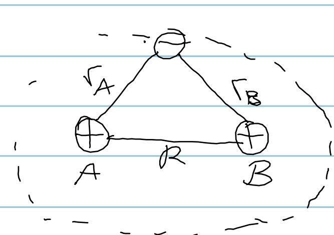




2-atom. Molekül

$R \approx 1\text{-}2\ \text{Å}$

$D_0 \approx 3\text{-}5\ \text{eV}$



<u>Hamilton-Op</u>

$$\hat{H} = -\frac{\hbar^2}{2M_A}\nabla_A^2 - \frac{\hbar^2}{2M_B}\nabla_B^2 - \frac{\hbar^2}{2m_e}\nabla^2 - \frac{e^2}{r_A} - \frac{e^2}{r_B} + \frac{e^2}{R}$$

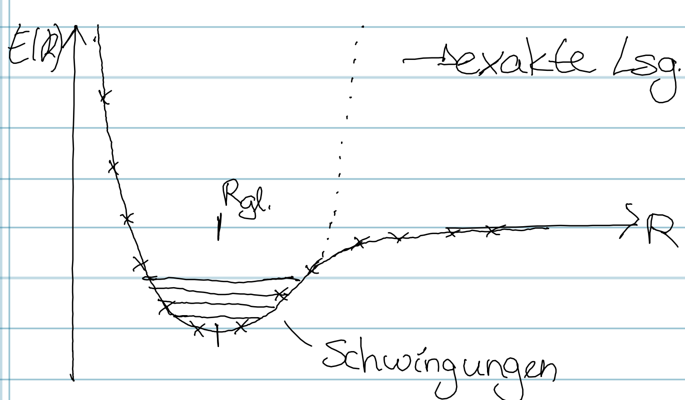
Dreikörperproblem

~~Born~~ Born-Oppenheimer-Näherung:

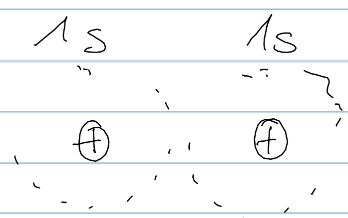
Bewegungen der Kerne (Schwingungen) können von den Bewegungen der Elektronen separiert werden, d.h. $E(R)$ lässt sich jeweils für einen festen Kernabstand R berechnen.

$$\boxed{\hat{H} = -\frac{\hbar^2}{2m_e}\nabla^2 - \frac{e^2}{r_A} - \frac{e^2}{r_B} + \frac{e^2}{R}}$$

$$\boxed{\hat{H}\,\Psi(R,r) = E(R)\,\Psi(R,r)}$$



Näherungslsg: MO-Theorie
Linearkombi. von Atomorb. (LCAO)



LCAO: $\boxed{\Psi = c_A\varphi_A + c_B\varphi_B}$

φ_A, φ_B = norm. WF H-Atom
c_A, c_B = Konstanten

$$|c_A|^2 = |c_B|^2 = |c|^2$$

$c_A = c_B$
$c_A = -c_B$

$$\boxed{\Psi = c(\varphi_A \pm \varphi_B)}$$

$$|\varphi_A + \varphi_B|^2 = |\varphi_A|^2 + |\varphi_B|^2 + \underbrace{2\varphi_A\varphi_B}_{\text{Erhöhung der } e^- \text{-Dichte zw. den Kernen}}$$

$$|\varphi_A - \varphi_B|^2 = |\varphi_A|^2 + |\varphi_B|^2 \underbrace{- 2\varphi_A\varphi_B}_{\text{Erniedrigung der } e^- \text{-Dichte zw. den Kernen}}$$