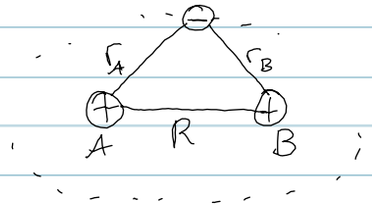
Vorlesung 13.12.2013

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

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

6 Moleküle und chemische Bindung

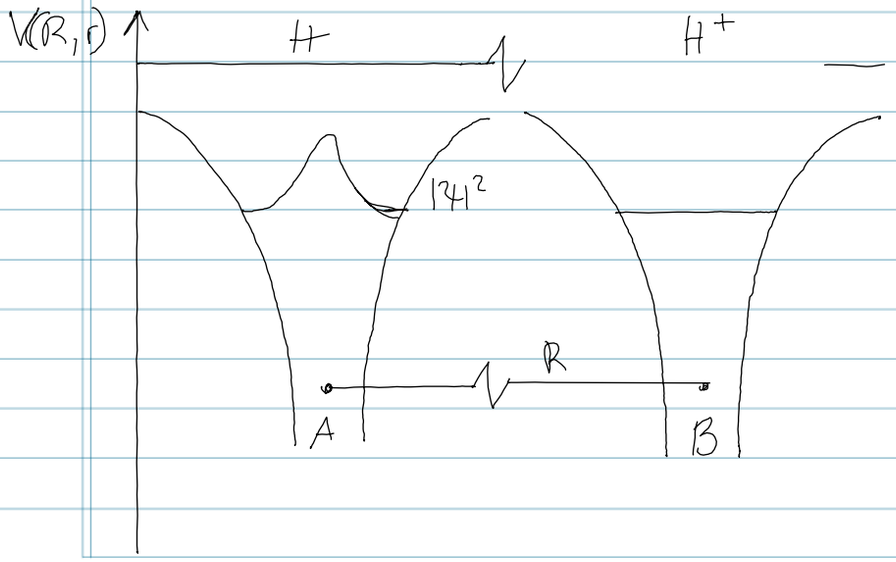
Wasserstoffmolekül-Ion H_2^+

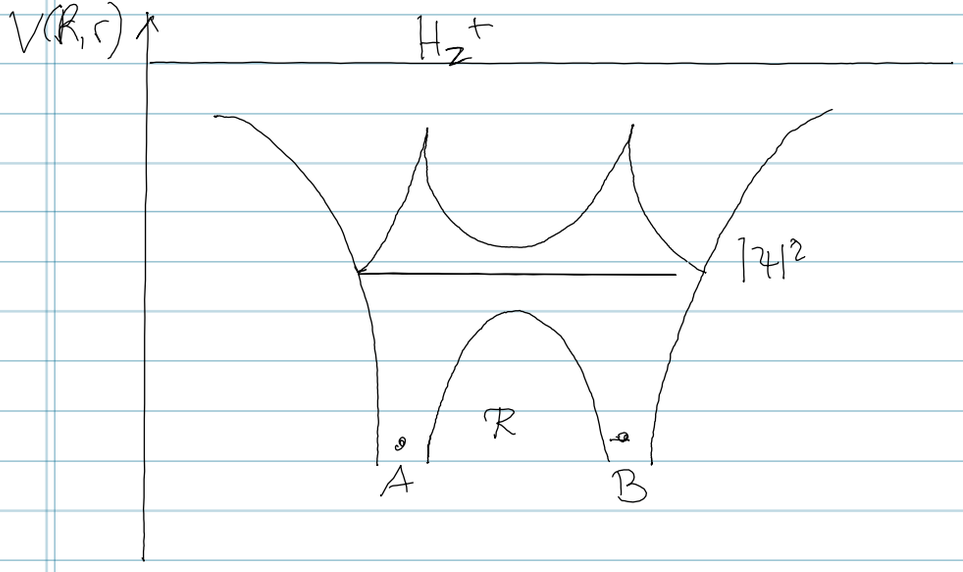


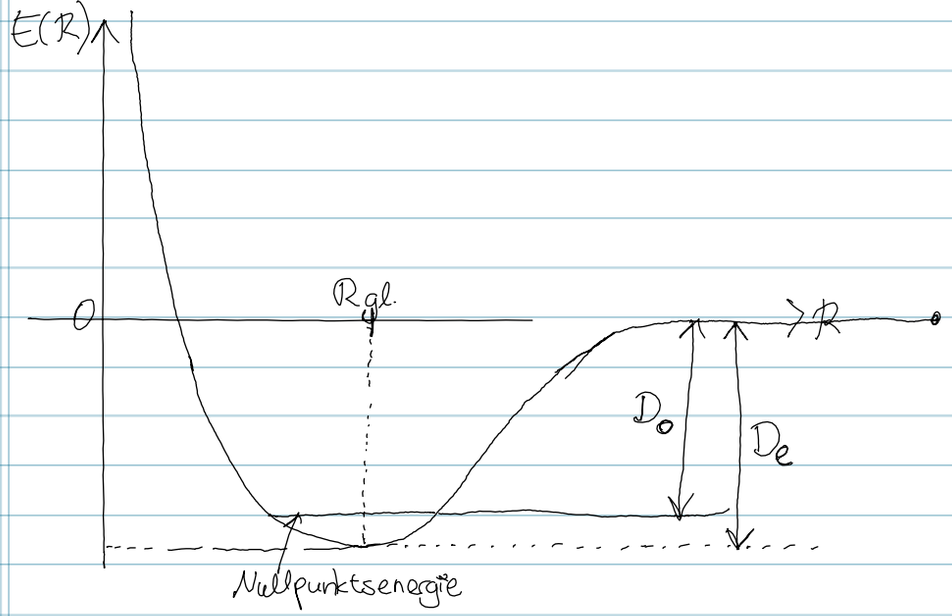
$R = 1,06 Å$

Bindungsenergie: 2,79eV

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



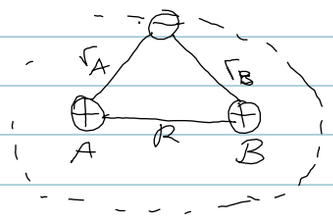




2-atom. Molekül

$R \approx 1\text{-}2$ Å

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



Hamilton-Op

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

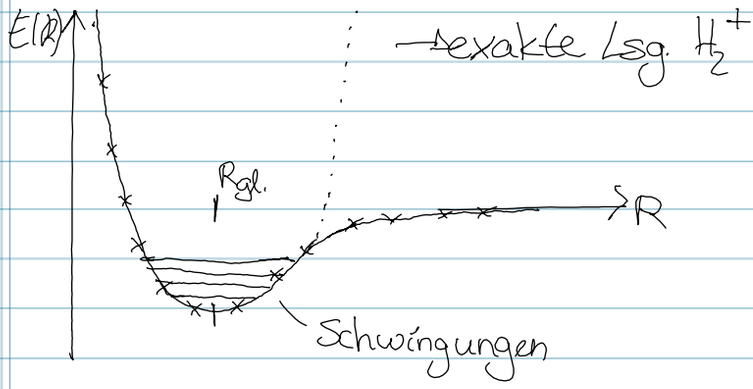
Dreikörperproblem

Born-Oppenheimer-Näherung:

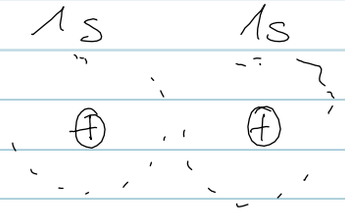
Bewegungen der Kerne (Schwingungen) können von den Bewegungen der Elektronen separiert werden, d.h. $E(R)$ lässt sich jeweils für einen festen Kernabstand R berechnen.

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

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



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



LCAO: $\psi = c_A\varphi_A + c_B\varphi_B$

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

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

$c_A = c_B$
$c_A = -c_B$

$$\psi = c(\varphi_A \pm \varphi_B)$$

$$|\varphi_A + \varphi_B|^2 = |\varphi_A|^2 + |\varphi_B|^2 + 2\varphi_A\varphi_B$$

Erhöhung der e^--Dichte zw. den Kernen

$$|\varphi_A - \varphi_B|^2 = |\varphi_A|^2 + |\varphi_B|^2 - 2\varphi_A\varphi_B$$

Erniedrigung der e^--Dichte zw. den Kernen