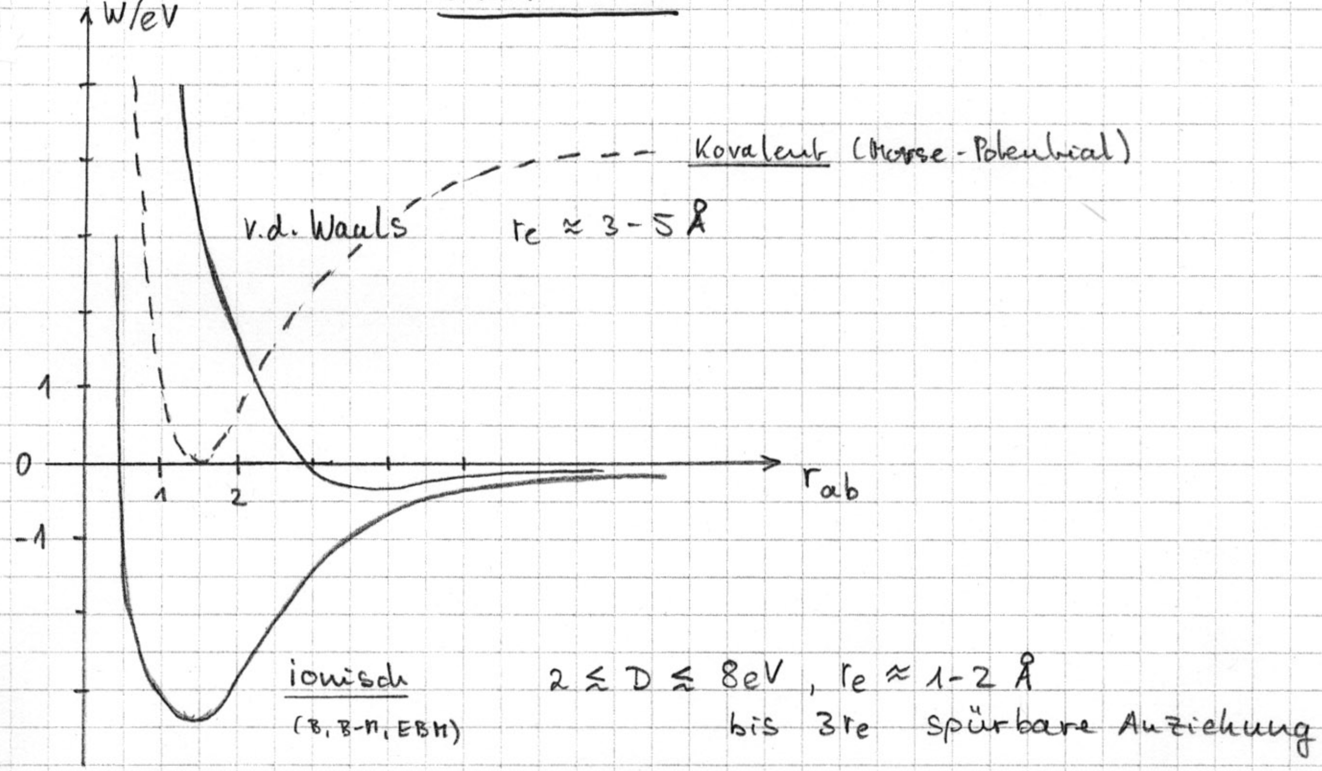
Blatt 12

42)



W/eV
1
0
-1
1
2
r_ab
Kovalent (Morse-Potential)
v.d. Waals
r_e ≈ 3-5 Å
ionisch
(B, B-M, EBM)
2 ≲ D ≲ 8eV , r_e ≈ 1-2 Å
bis 3r_e spürbare Anziehung

43) erweitertes Born – Mayer – Potential

$$W(r) = -\frac{e^2 z^2}{4\pi\varepsilon_0 r} + \beta_1 e^{-r/\varrho_1} - \frac{d}{r^6} \qquad (z=1)$$

$\beta_1, \varrho_1, d \quad \rightarrow \quad 3$ Konstanten

a)
$$\frac{dW}{dr} = +\frac{e^2}{4\pi\varepsilon_0 r^2} - \frac{\beta_1}{\varrho_1} e^{-r/\varrho_1} + \frac{6d}{r^7}$$

$$\frac{d^2W}{dr^2} = -\frac{2e^2}{4\pi\varepsilon_0 r^3} + \frac{\beta_1}{\varrho_1^2} e^{-r/\varrho_1} - \frac{42\,d}{r^8}$$

Gleichgewichtsabstand: $\frac{dW}{dr} \stackrel{!}{=} 0$ für r_e

$$\Rightarrow \underline{\frac{e^2}{4\pi\varepsilon_0 r_e^2} - \frac{\beta_1}{\varrho_1} e^{-r_e/\varrho_1} + \frac{6d}{r_e^7} = 0}$$

Dissoziationsenergie:

$$\underline{D_e = W(r \rightarrow \infty) - W(r_e) = +\frac{e^2}{4\pi\varepsilon_0 r_e} - \beta_1 e^{-r_e/\varrho_1} + \frac{d}{r_e^6}}$$

Federkonstante:

$$\underline{k_e = \left(\frac{d^2W}{dr^2}\right)_{r=r_e} = -\frac{2e^2}{4\pi\varepsilon_0 r_e^3} + \frac{\beta_1}{\varrho_1^2} e^{-r_e/\varrho_1} - \frac{42\,d}{r_e^8}}$$

b) $r \rightarrow 0 \quad \rightsquigarrow \quad W(r) \rightarrow -\infty$

$r \rightarrow \infty \quad \rightsquigarrow \quad W(r) \rightarrow 0$

c) LiF: $d = 2.68\,\text{eV}\,\text{Å}^6$, $\varrho_1 = 0{,}308\,\text{Å}$; $\beta_1 = 895\,\text{eV}$

$$W(r) = -\frac{14{,}40\,\text{eV}\cdot\text{Å}}{r} + 895\,\text{eV}\, e^{-r/0{,}308\,\text{Å}} - \frac{2{,}68\,\text{eV}\,\text{Å}^6}{r^6}$$

$r_e = ?$

$$\frac{14{,}40\,\text{eVÅ}}{r_e^2} - \frac{895\,\text{eV}}{0{,}308\,\text{Å}} e^{-r_e/0{,}308\,\text{Å}} + \frac{6\cdot 2{,}68\,\text{eV}\,\text{Å}^6}{r_e^7} = 0$$

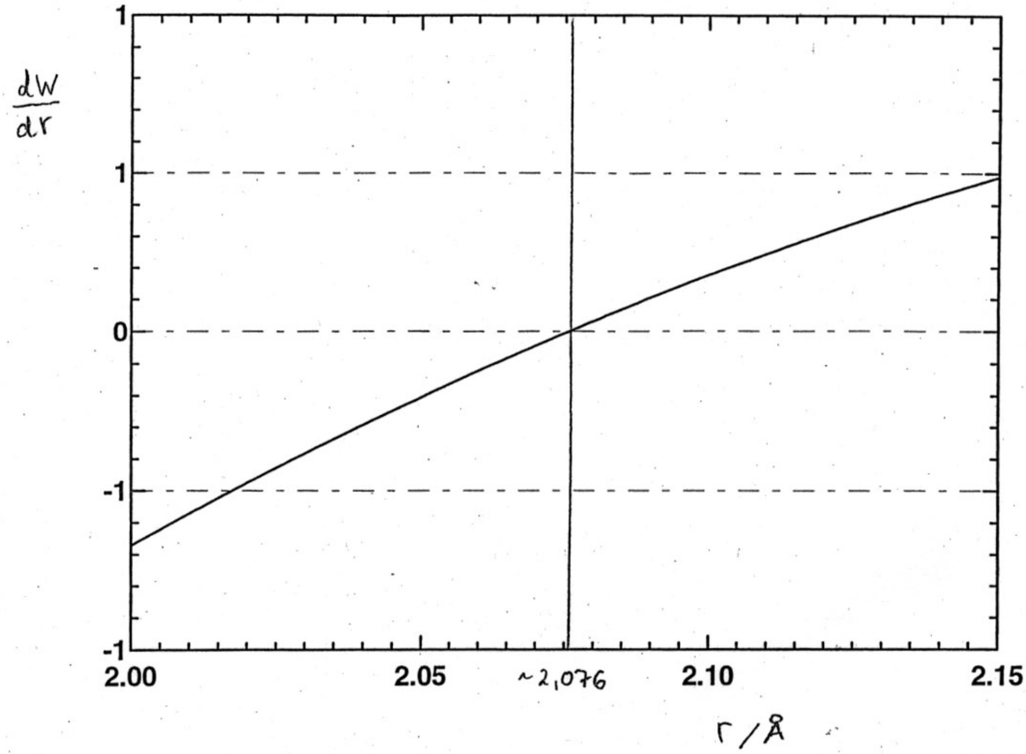
$$\frac{14{,}40}{r_e^2} - 2905{,}8\, e^{-r_e/0{,}308} + \frac{16{,}08}{r_e^7} \stackrel{!}{=} 0$$

graphische Lösung: $\underline{\underline{r_e = 2{,}076\,\text{Å}}}$

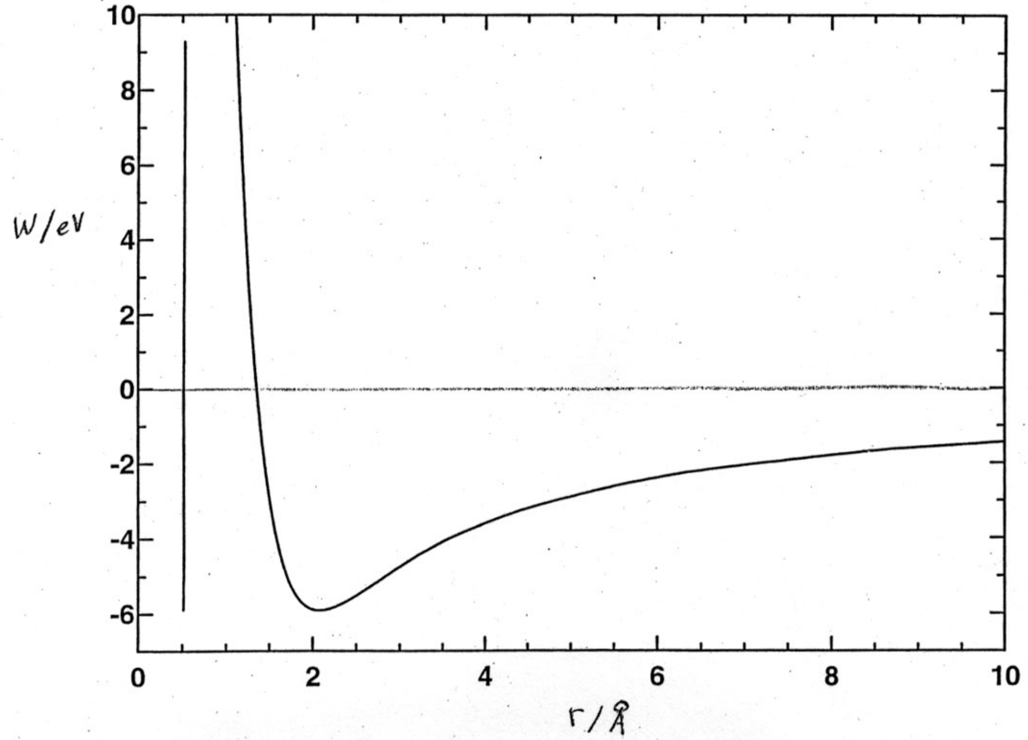
damit: $\underline{\underline{D_e = 5{,}91 \text{ eV}}}$

$\underline{\underline{k_e = 7{,}61 \ \frac{\text{eV}}{\text{Å}} = 121{,}9 \ \frac{\text{N}}{\text{m}}}}$

Skizze zur Bestimmung von r_e:

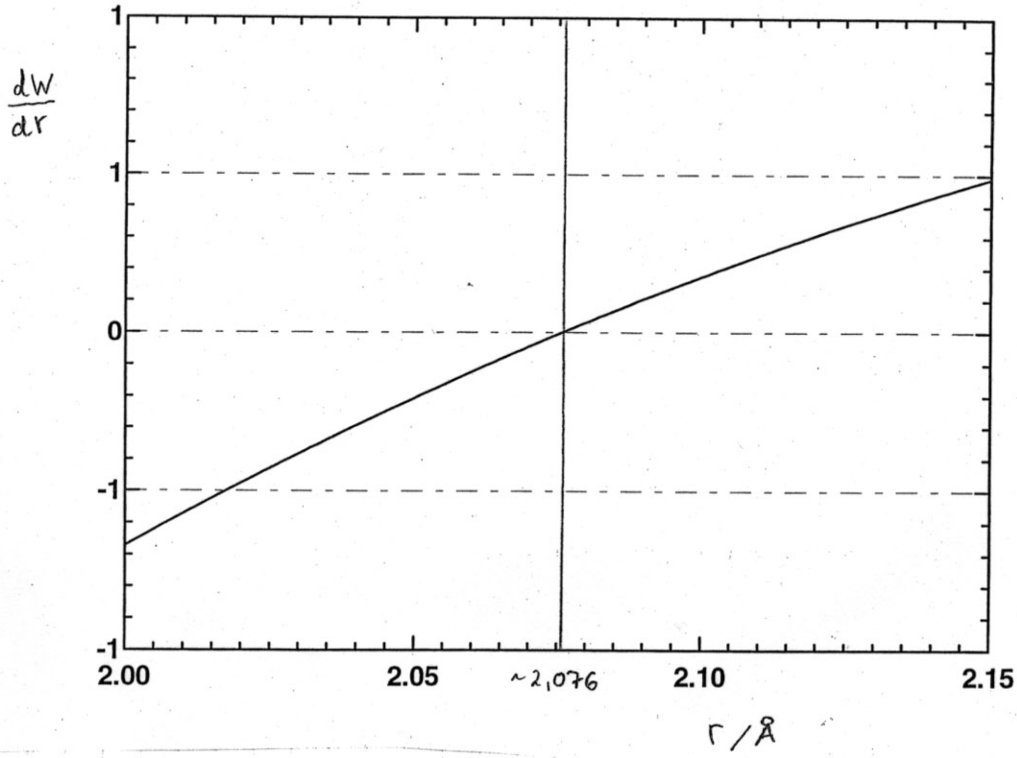


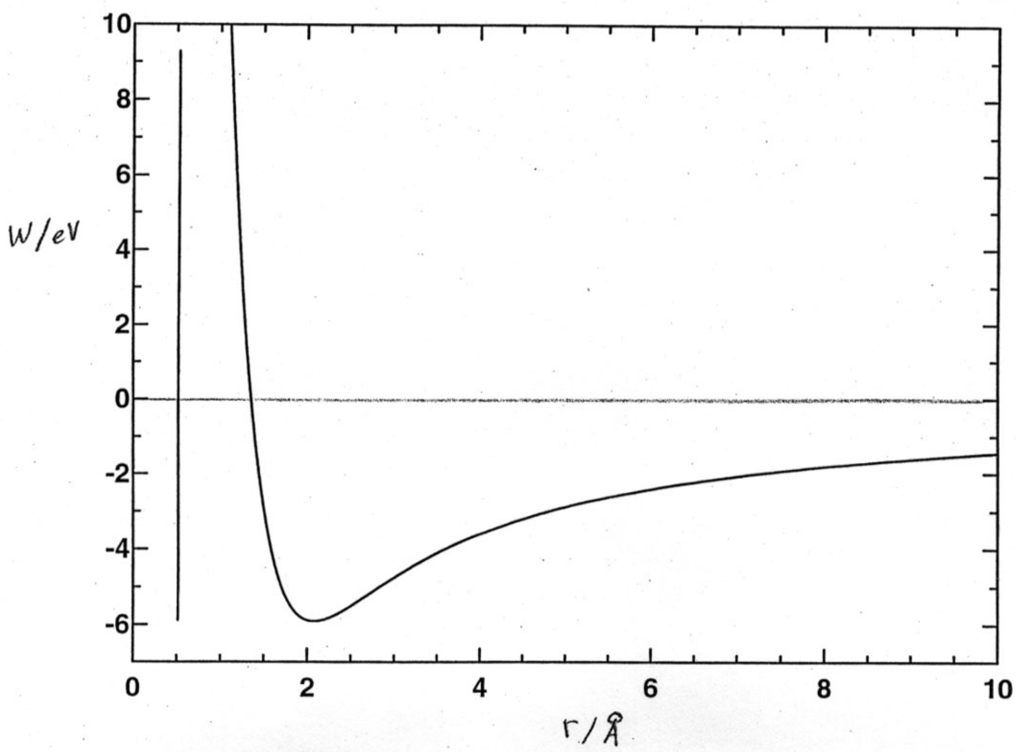
Skizze des erw. B-M-Potentials:



damit: $\underline{\underline{D_e = 5{,}91\ \mathrm{eV}}}$

$\underline{\underline{k_e = 7{,}61\ \frac{\mathrm{eV}}{\mathrm{Å}} = 121{,}9\ \frac{\mathrm{N}}{\mathrm{m}}}}$





44)

Morsepotential : $W = D\left(1 - e^{-a(r-r_0)}\right)^2$

r_e : $\left.\frac{dW}{dr}\right|_{r=r_e} \overset{!}{=} 0$

$$\frac{dW}{dr} = 2D\left(1 - e^{-a(r-r_0)}\right) e^{-a(r-r_0)}\, a \overset{!}{=} 0$$

$$\Rightarrow e^{-a(r-r_0)} \overset{!}{=} 1 \quad \Rightarrow \quad r_e = r_0$$

allgemein: $\omega_0 = \sqrt{\frac{k}{m}}$

$k = \left.\frac{d^2W}{dr^2}\right|_{r=r_e}$ aus Aufg. 43

$$\frac{d^2W}{dr^2} = 2D\left(a\, e^{-a(r-r_0)}\right) a\, e^{-a(r-r_0)} - 2D\left(1 - e^{-a(r-r_0)}\right) a^2 e^{-a(r-r_0)}$$

$$k \overset{r_e = r_0}{=} 2Da^2 - 2D(1-1)\,a^2 = 2Da^2$$

$\Rightarrow \omega^2 = \frac{2Da^2}{\mu}$ mit effektiver Masse $\mu = \frac{m_1 \cdot m_2}{m_1 + m_2}$