Abschn. 5.5 Numerische Durchführung

DFT: $E_g = E[n]$, $n(\vec{r})$ Elektronendichte

aus Einelektronenpotenzial $v(\vec{r}) = v(\vec{r}, \vec{R}_1, \vec{R}_2, \ldots \vec{R}_N)$

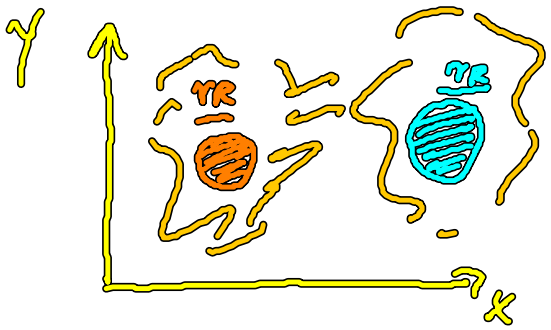
$E_g(\vec{R}_1, \vec{R}_2, \ldots \vec{R}_N) \Longrightarrow$

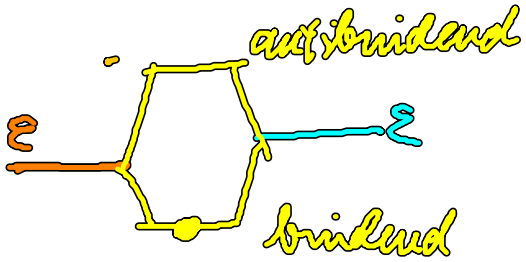
1) Molekülstruktur Min. E_g: $\frac{\partial E_g}{\partial \vec{R}_1} = 0$; $\frac{\partial E_g}{\partial \vec{R}_2} = 0$, ... $\frac{\partial E_g}{\partial \vec{R}_N} = 0$

Verfahren der konjugierten Gradienten

2) $\frac{\partial E_g}{\partial \vec{R}_j} = -\vec{F}_j$ aus $M_j \ddot{\vec{R}}_j(t) = \vec{F}_j$; $\ddot{\vec{R}}_j(t) = \frac{1}{M_j}\vec{F}_j = -\frac{1}{M_j}\frac{\partial E_g}{\partial \vec{R}_j}$

Δt mit $\ddot{\vec{R}}_j(t) \approx \frac{1}{\Delta t^2}\left(\vec{R}_j(t-\Delta t) - 2\vec{R}_j(t) + \vec{R}_j(t+\Delta t)\right)$





Kapitel 6 Anwendungen der DFT