


Center for
Molecular
Modeling

Computational Materials Physics

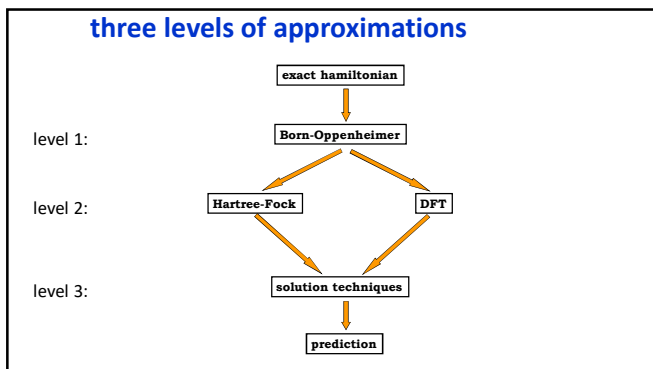


Department of
Materials Science
and Engineering

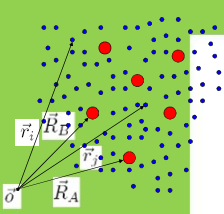
the external potential

Stefaan.Cottenier@ugent.be
Technologiepark 903, Zwijnaarde

<http://molmod.ugent.be>
<http://www.ugent.be/ea/dmse/en>
my talks on Youtube: <http://goo.gl/P2b1Hs>



which interactions ?



$$\begin{aligned}
& \sum_A -\frac{\hbar^2 \nabla_A^2}{2M_A} \\
& + \sum_i -\frac{\hbar^2 \nabla_i^2}{2m_i} \\
& + \frac{1}{2} \frac{1}{4\pi\epsilon_0} \sum_{A \neq B} \frac{+e^2 Z_A Z_B}{|\vec{R}_A - \vec{R}_B|} \\
& + \frac{1}{2} \frac{1}{4\pi\epsilon_0} \sum_{i,j} \frac{-e^2}{|\vec{r}_i - \vec{r}_j|} \\
& + \frac{1}{4\pi\epsilon_0} \sum_{i,A} \frac{-e^2 Z_A}{|\vec{r}_i - \vec{R}_A|}
\end{aligned}$$

N

\vec{R}_A

$$+ \frac{1}{4\pi\epsilon_0} \sum_{i,A}^N \frac{-e^2 Z_A}{|\vec{r}_i - \vec{R}_A|}$$

energy of N electrons
in the electric potential
provided by
a given set of nuclei at \vec{R}_A

$$+ \frac{1}{4\pi\epsilon_0} \sum_{i,A}^N \frac{-e^2 Z_A}{|\vec{r}_i - \vec{R}_A|}$$

energy of N electrons
in the **electric potential**
provided by
a given set of nuclei at \vec{R}_A



external potential

$$V_{ext}(\vec{r}) = + \frac{1}{4\pi\epsilon_0} \sum_A \frac{eZ_A}{|\vec{r} - \vec{R}_A|}$$



electric potential
provided by
a given set of nuclei at \vec{R}_A



external potential
