

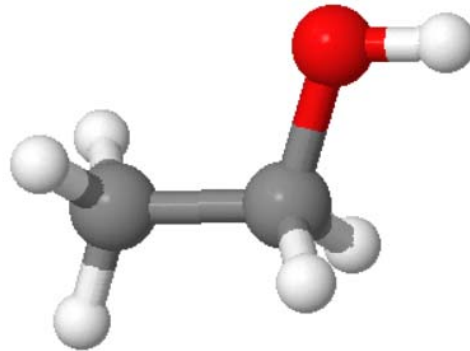
# Molecular and Solid State Physics

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# Goal

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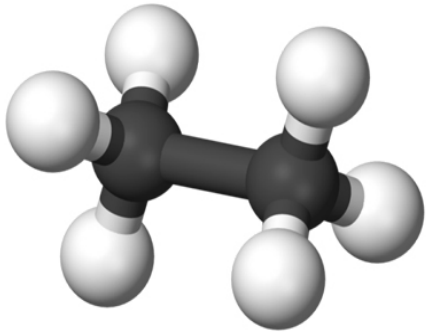
From the microscopic structure



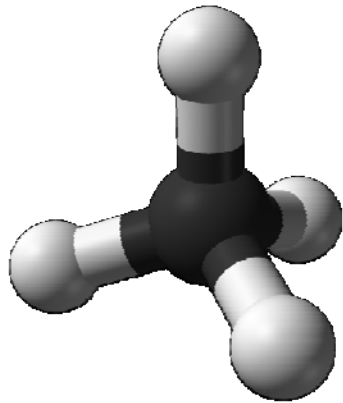
calculate any property of any molecule or any solid.

# Molecules

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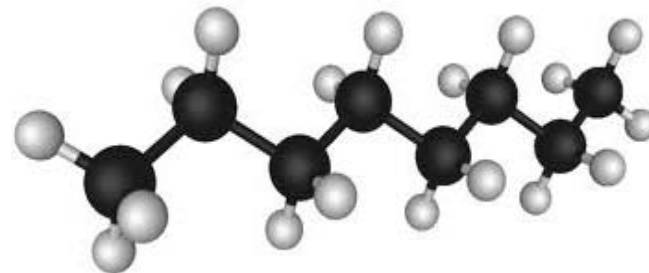
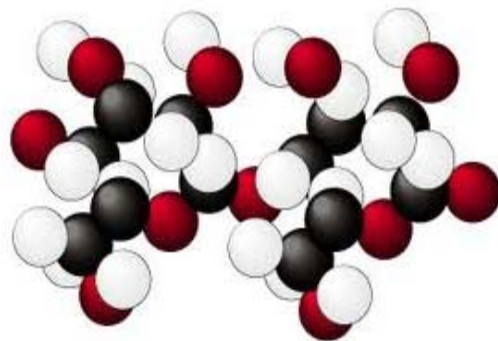


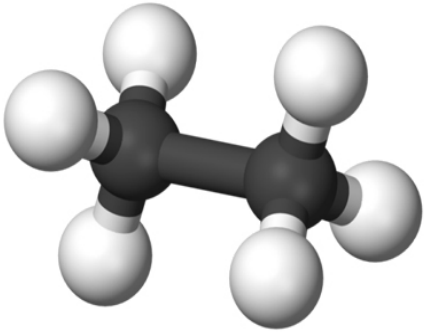
There are billions of useful molecules.



Acids, esthers, alkanes, ...

Biological molecules: DNA, RNA, proteins





# Molecules

Every property of a molecule can be calculated using multi-particle quantum mechanics.

$$H_{\text{mp}} = - \sum_i \frac{\hbar^2}{2m_e} \nabla_i^2 - \sum_a \frac{\hbar^2}{2m_a} \nabla_a^2 - \sum_{a,i} \frac{Z_a e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{r}_a|} + \sum_{i<j} \frac{e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{r}_j|} + \sum_{a<b} \frac{Z_a Z_b e^2}{4\pi\epsilon_0 |\vec{r}_a - \vec{r}_b|}$$



We will calculate:

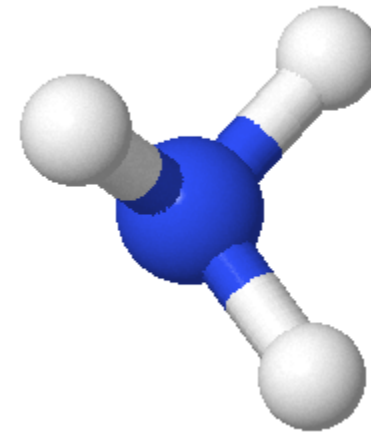
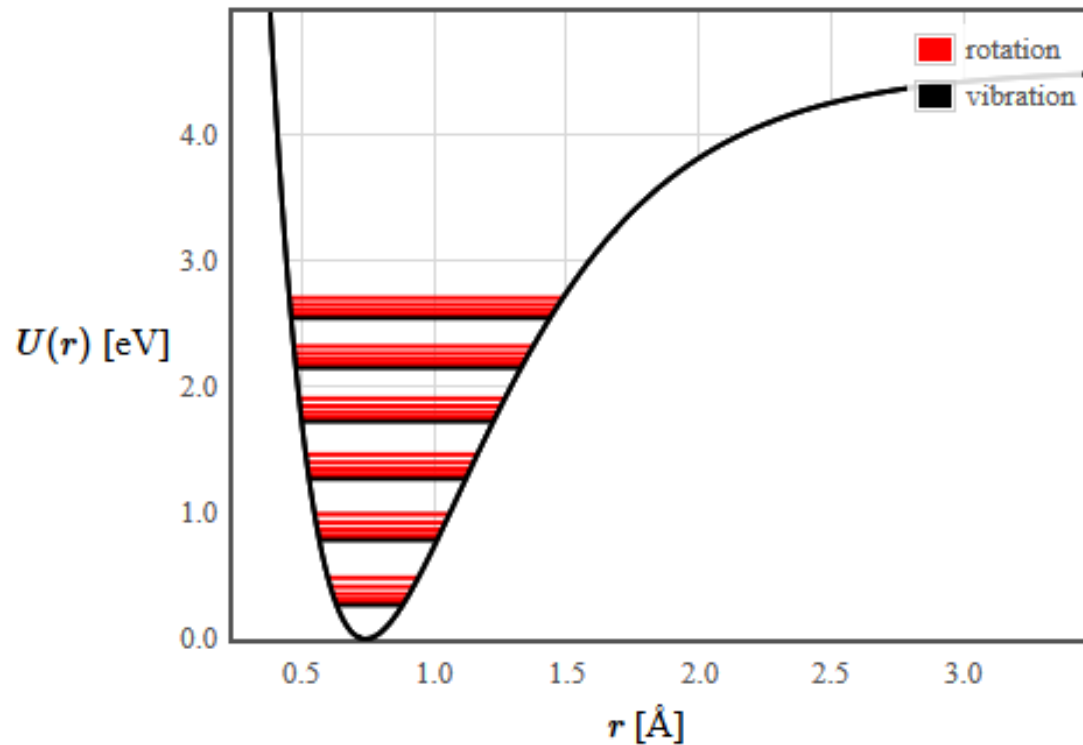
- bond length
- bond strength
- molecular energy levels



# Molecules

$$H_{\text{mp}} = - \sum_i \frac{\hbar^2}{2m_e} \nabla_i^2 - \sum_a \frac{\hbar^2}{2m_a} \nabla_a^2 - \sum_{a,i} \frac{Z_a e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{r}_a|} + \sum_{i<j} \frac{e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{r}_j|} + \sum_{a<b} \frac{Z_a Z_b e^2}{4\pi\epsilon_0 |\vec{r}_a - \vec{r}_b|}$$

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$



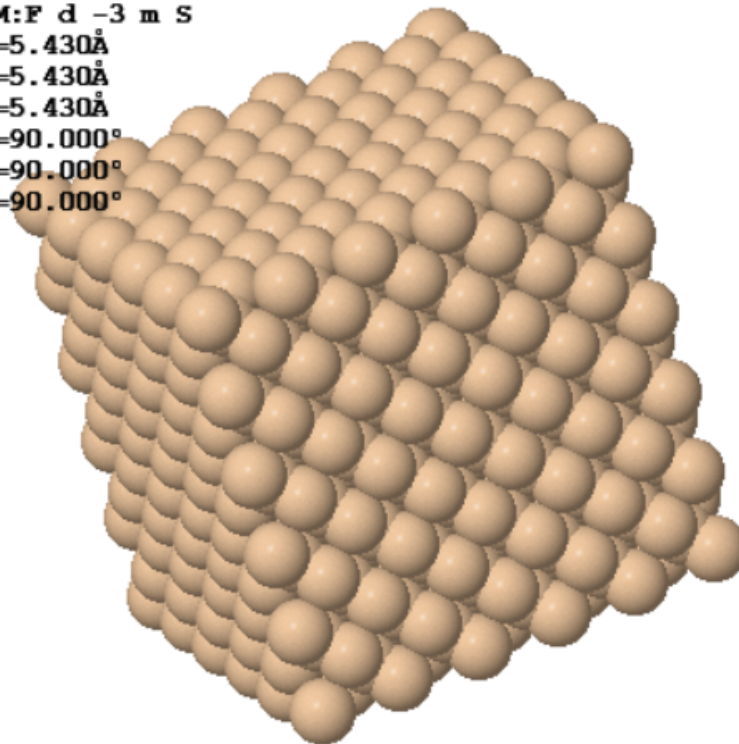
Bond length: 0.74144 Å.  
 Dissociation energy: 4.52 eV.

# Solids

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Solids are large molecules

HM:F d -3 m S  
a=5.430Å  
b=5.430Å  
c=5.430Å  
 $\alpha=90.000^\circ$   
 $\beta=90.000^\circ$   
 $\gamma=90.000^\circ$



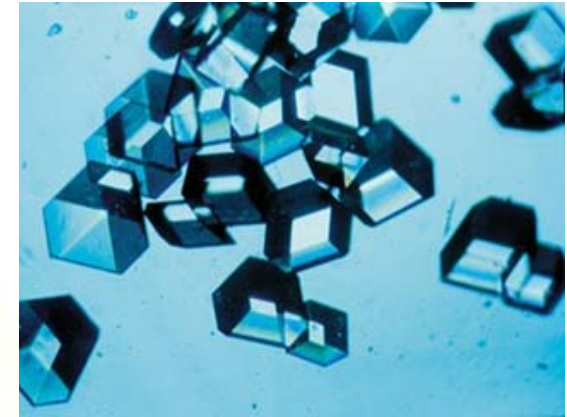
# Crystal = periodic arrangement of atoms



Gallium crystals



quartz



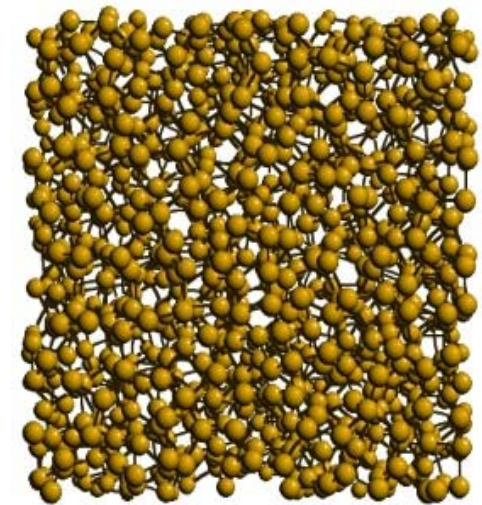
Insulin crystals



amorphous metal



glass

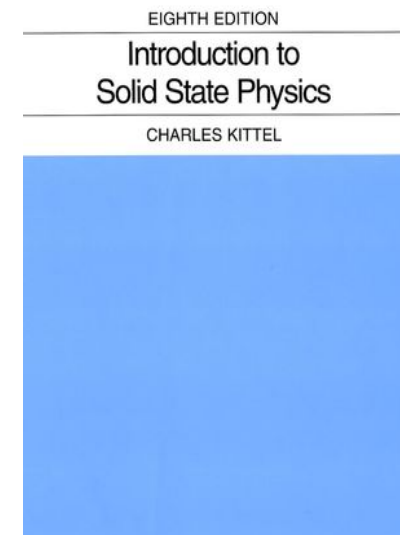
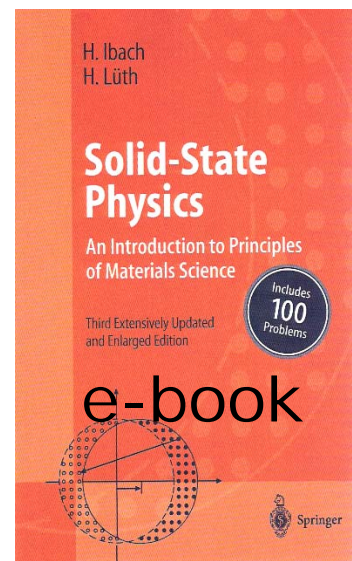
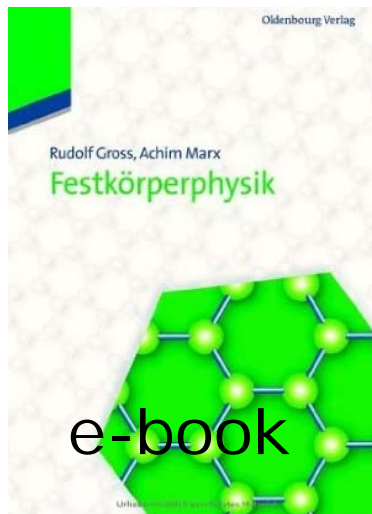
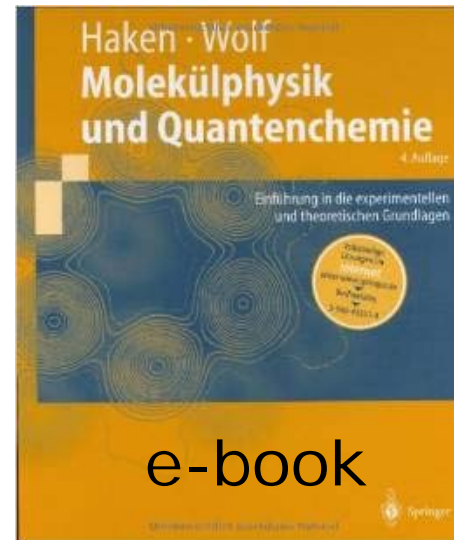


amorphous silicon

<http://www.wikipedia.org>

[http://www.pmc.umontreal.ca/~mousseau/site\\_an/uploads/Main/si1000.jpg](http://www.pmc.umontreal.ca/~mousseau/site_an/uploads/Main/si1000.jpg)

# Books





<http://www.if.tugraz.at/ss1.html>



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PHY.F20 Molecular and Solid State Physics

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