Center for Molecular Modeling

Computational Materials Physics

Department of Materials Science and Engineering

solids as quantum systems

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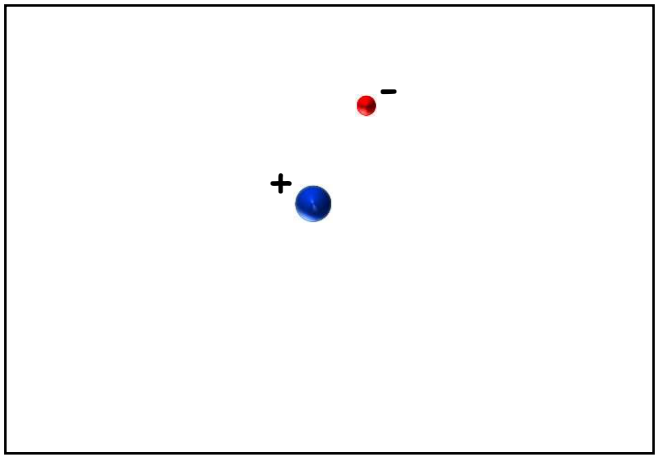
http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs

Before watching this video,
it might be useful to pause it for a while
and to ponder the following task :

Write down **your** definition of a solid.

You may want
to pause the video
in order to think about
the previous question.

Proceed
once you have
your answer ready.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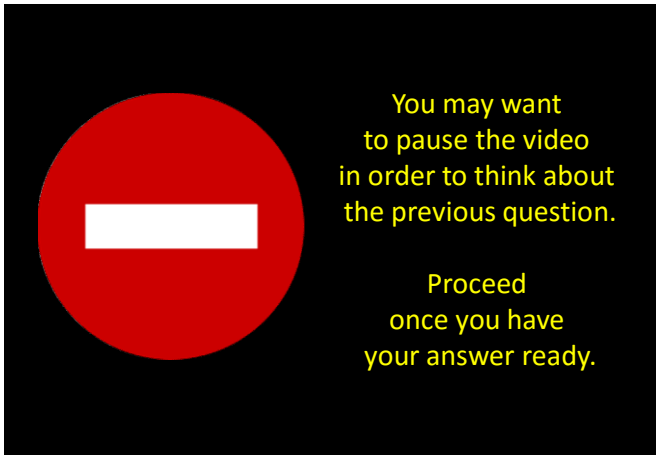
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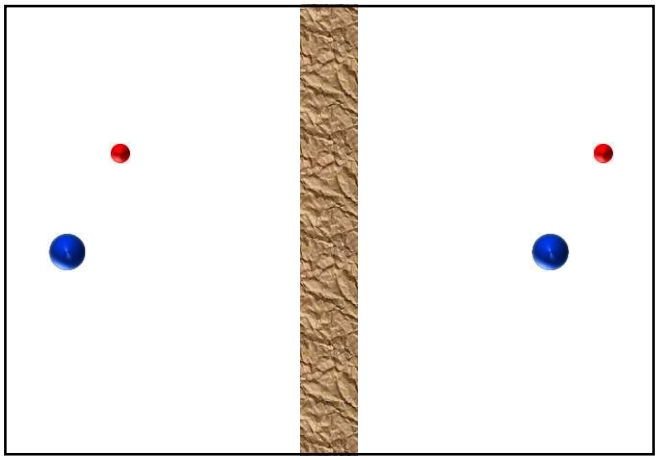

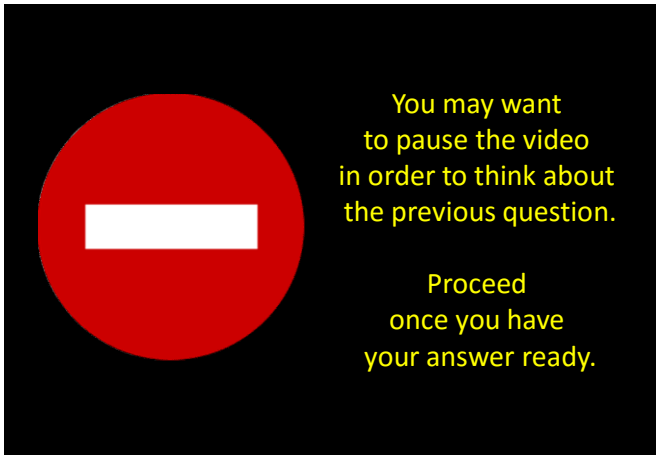
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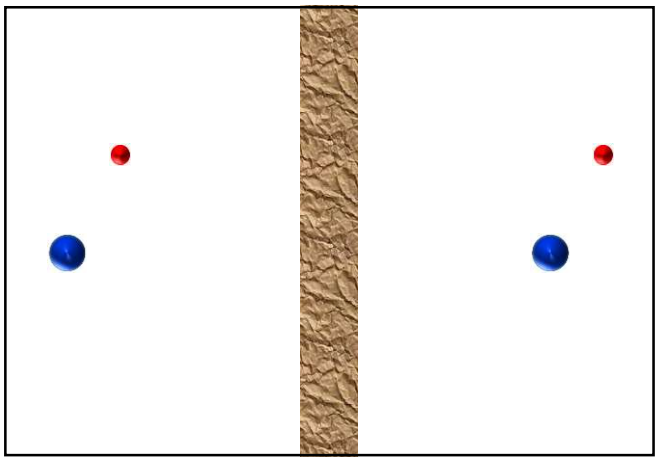
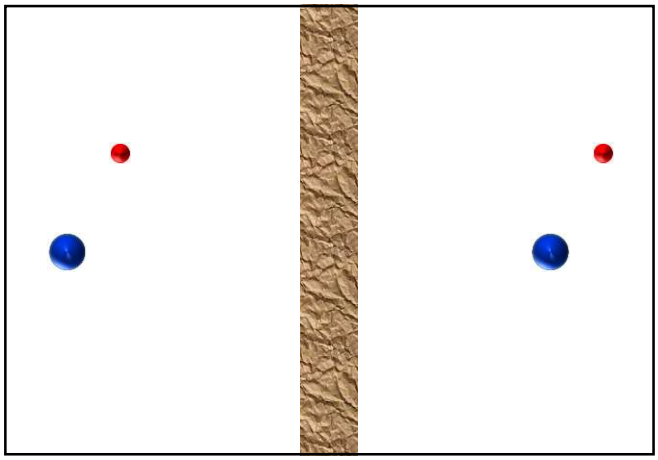
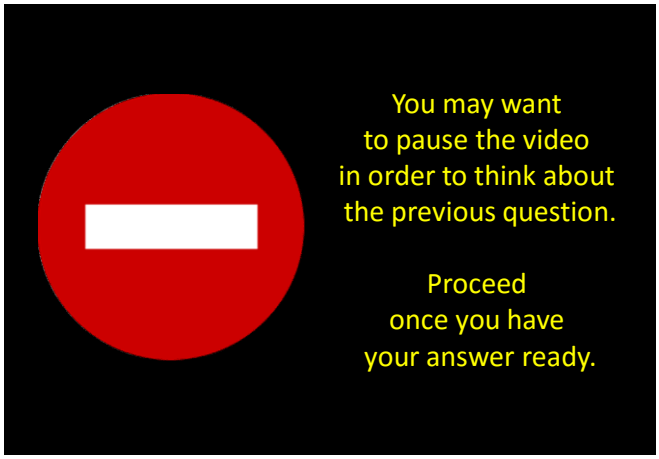
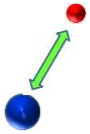




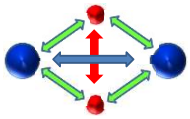


1+1≠2

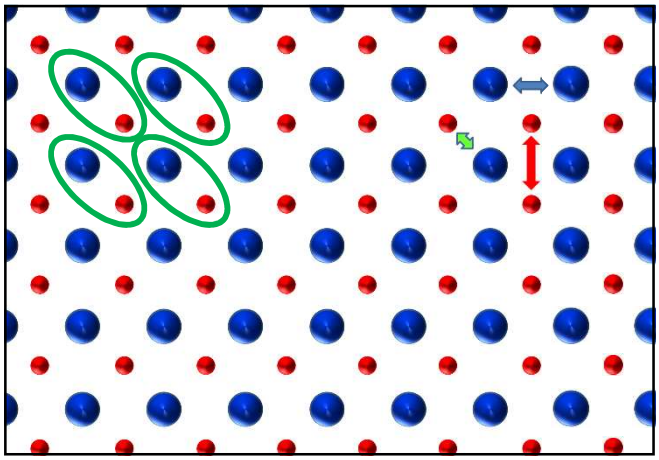
e-n interaction



e-n interaction
n-n interaction
e-e interaction

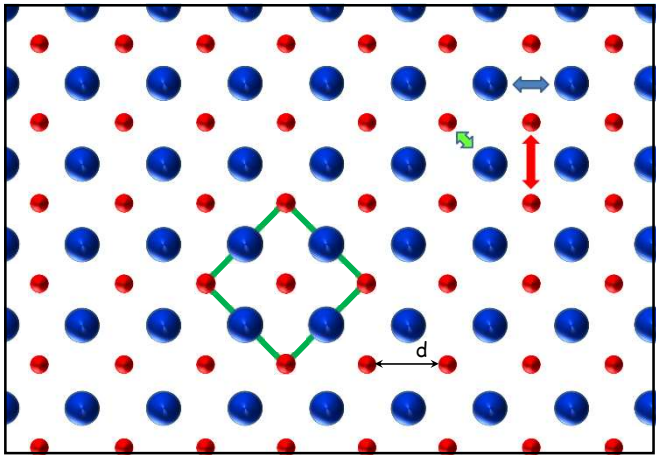


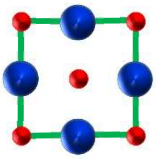
qualitatively different systems !



Definition of a solid (part 1)

spoiler prevention





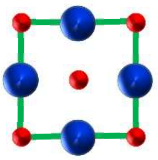
Coulomb interaction energy per cell
(nn+nnn pairs only) :

?

(try to find out)

Nice exercise,
yet it takes some time.
You can do it
either now or later.

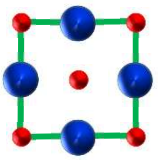
No harm if
you proceed
with the video
right away.



Coulomb interaction energy per cell
(nn+nnn pairs only) :

$$E_{tot} = \underbrace{\left(-3\sqrt{2}+2\right)}_{\approx -2.24} \frac{e^2}{d}$$

also known as **total energy :**
(very important quantity,
it will appear often in this course)



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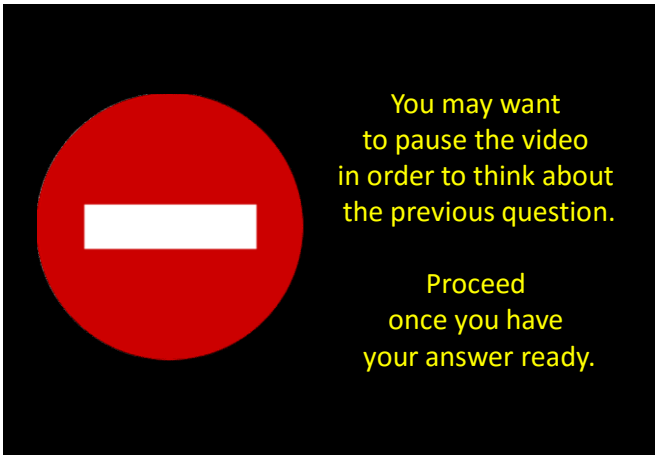
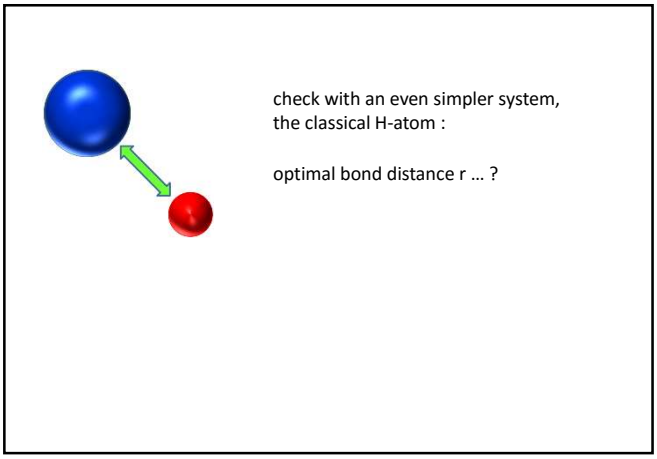
- negative ➔ crystal is bound
- optimal lattice parameter d…?





Definition of a solid (full)

spoiler prevention

Definition of a solid (full)

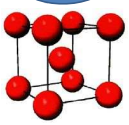
spoiler prevention

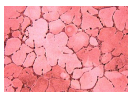
Crystal structure determines properties of the solid

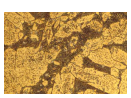
Yet, there is more….

this course (mainly)

properties of a material = crystal structure + microstructure







microstructure =
- type and number of defects
- grain size
- grain orientation
- …