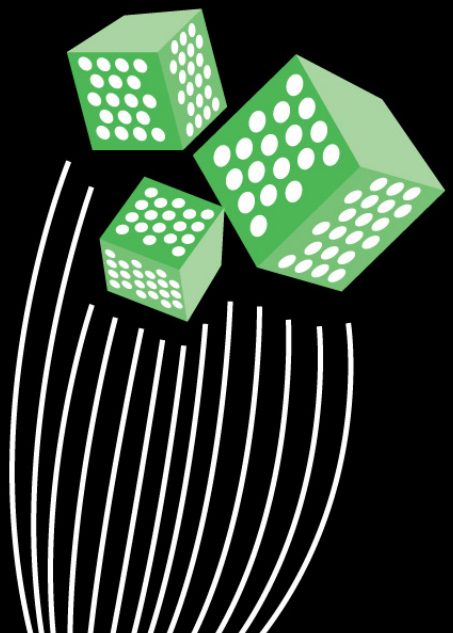
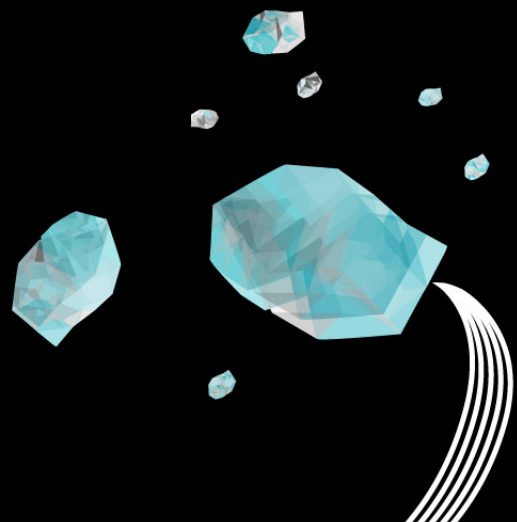
UNIVERSITY OF TWENTE.

MESA+
INSTITUTE FOR NANOTECHNOLOGY

Computational Physics

Claudia Filippi (CCP), Geert Brocks (CMS),
Jeroen Verschuur (SLT)





What is Computational Physics ?

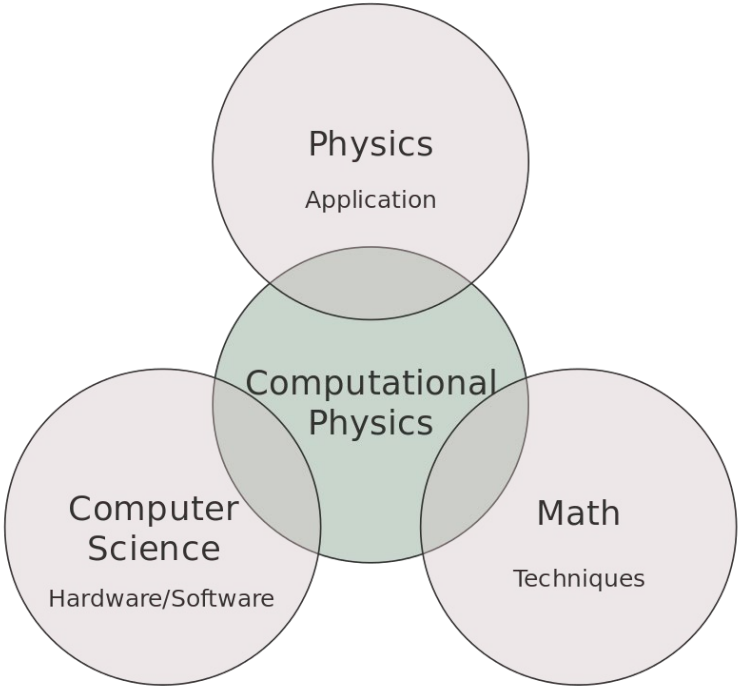
- physics on the computer
- numerical calculations to solve physics equations
- computational experiments:

  generate data, analyze, make/verify model

- connects physics to

  numerical mathematics and

  computer science



Organization Computational Physics

Book: lecture notes

Form: - practical work (programming & analysis)

- project assignments (4)

H&S ware: (your own) laptop & python/matlab

Meetings: 2 X per week afternoon/morning

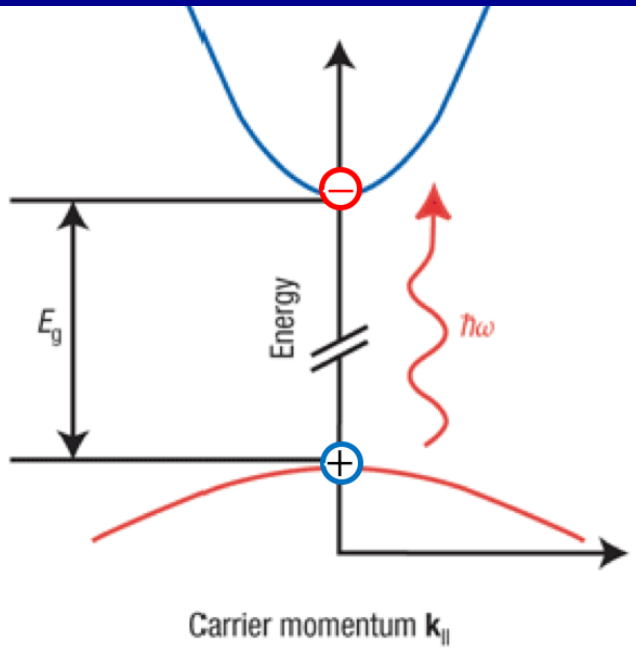
Assessment: written report for each assignment

Philosophy: no black boxes (think inside of the box)

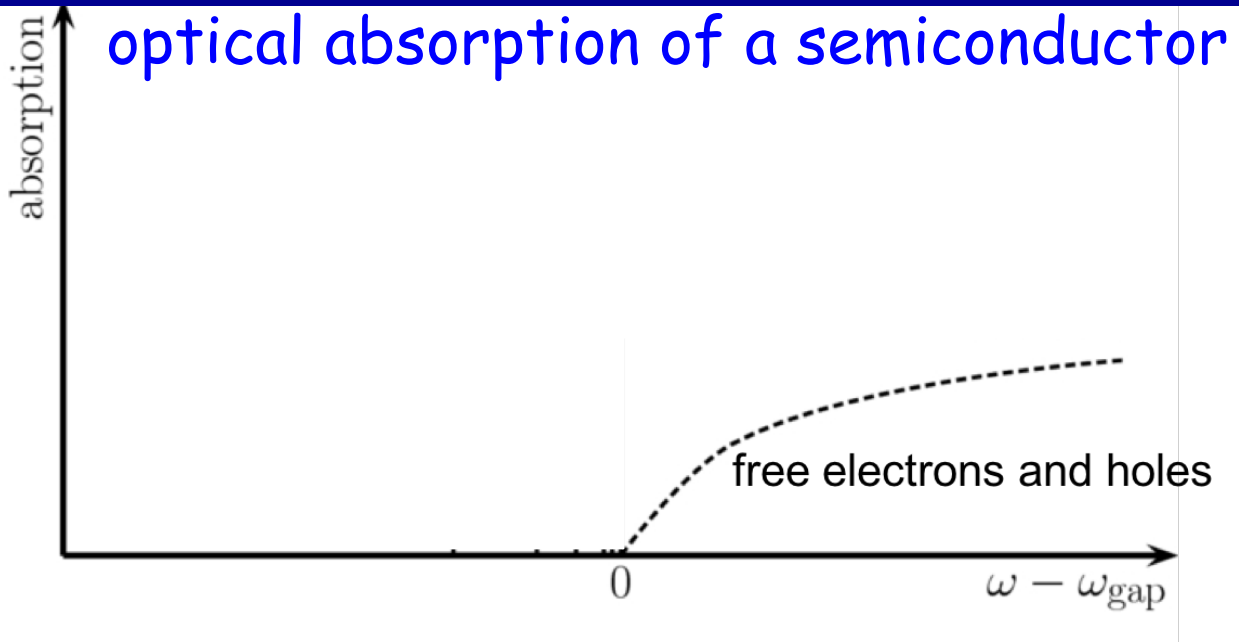
For whom? - affinity with physical modeling

- affinity with computer work

Project 1: Excitons $\hat{H}\,\psi(\mathbf{r}) = E\,\psi(\mathbf{r})$

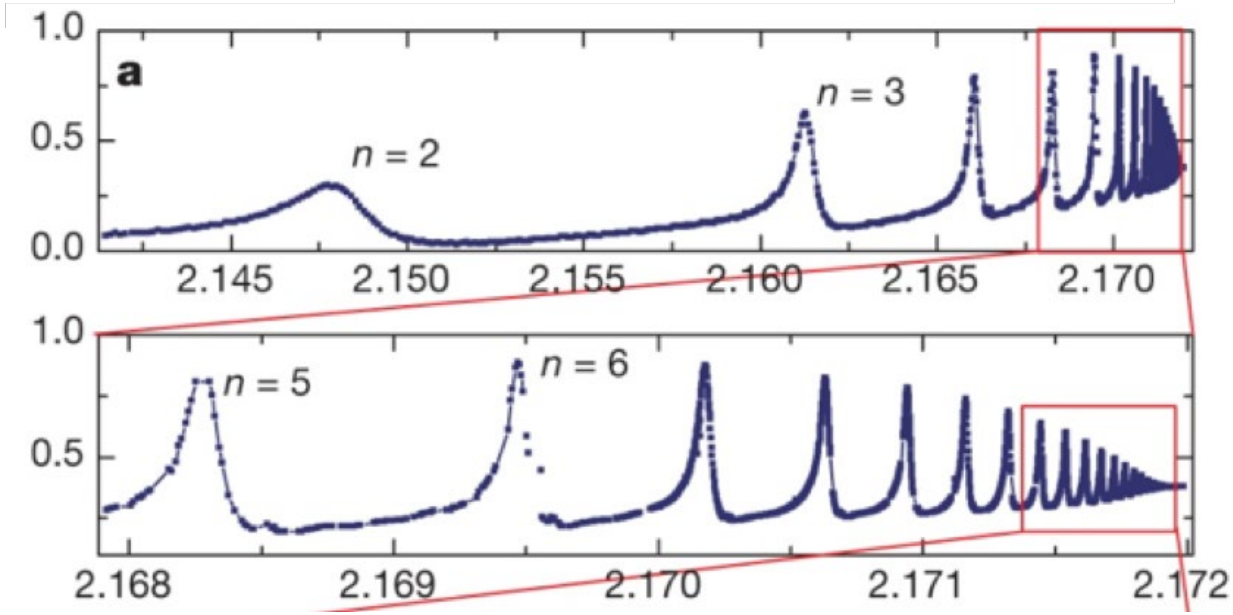


optical absorption of a semiconductor

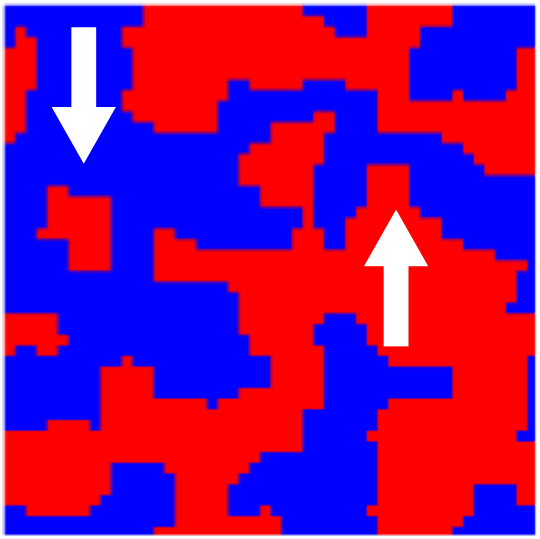


Excitons in Cu_2O

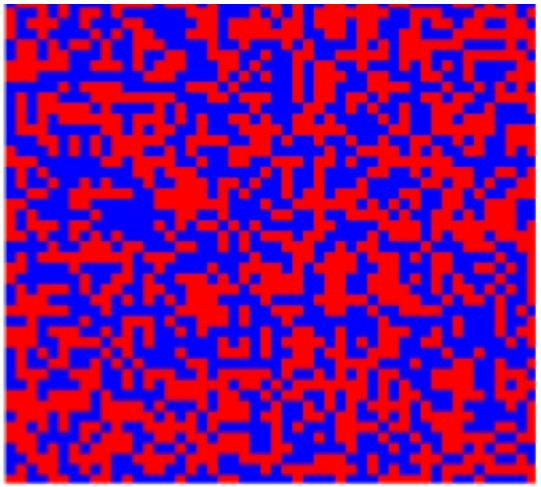
Kazimierczuk et al,
Nature 514, 343 (2014)



Project 2: magnetism $\bar{E} = \Sigma_i E_i e^{-E_i/k_B T} / Z$

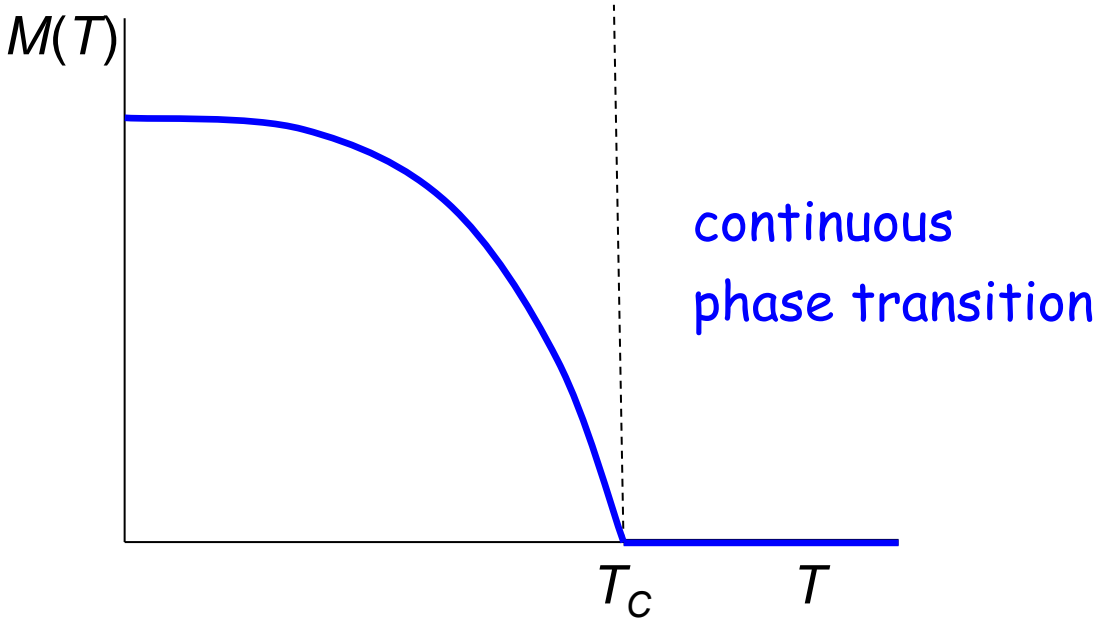


$T \ll T_C$



$T \gg T_C$

magnetization



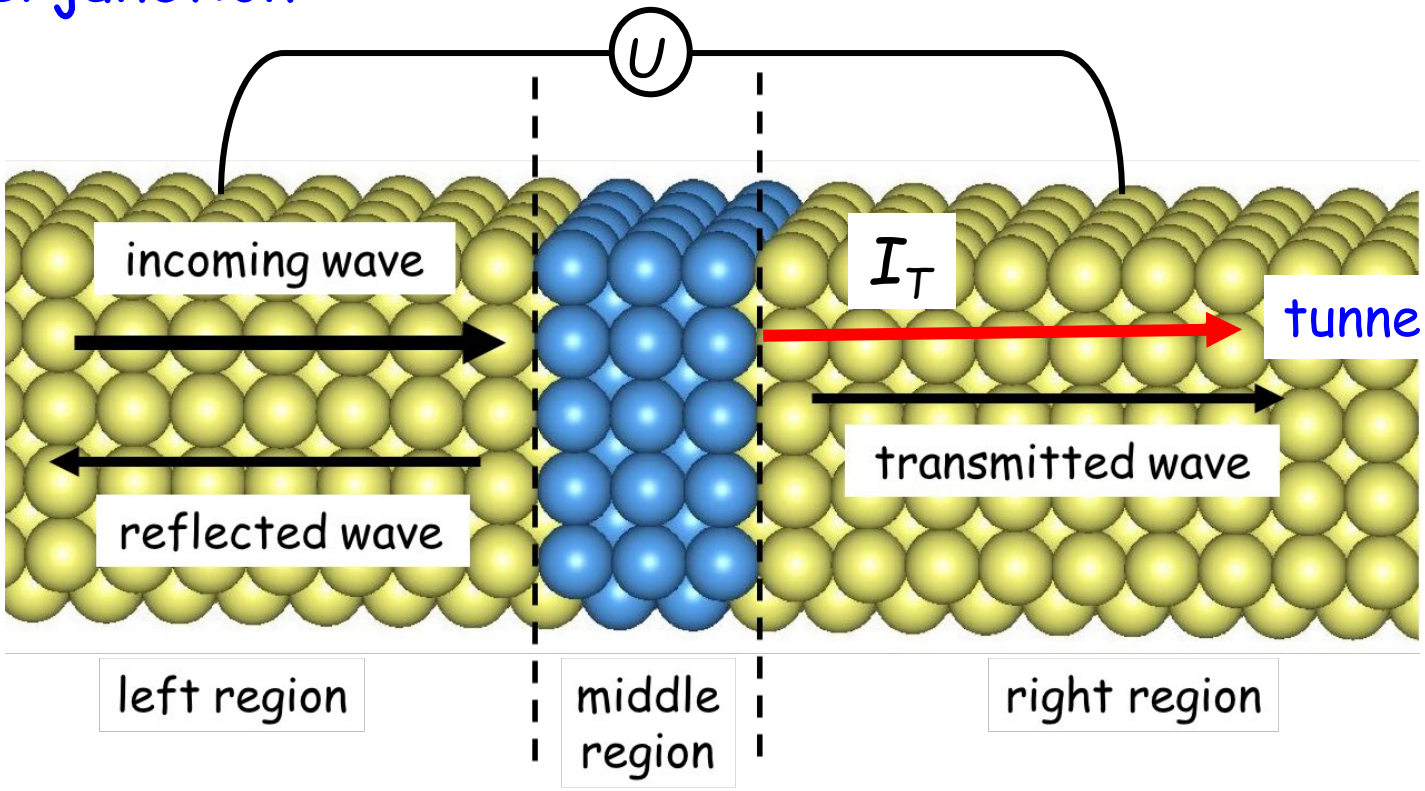
continuous
phase transition

Monte Carlo
simulation

rolling the dice
and assembling statistics

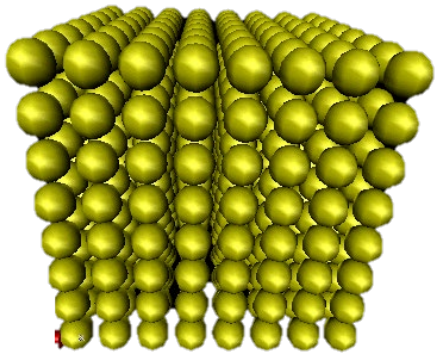
Project 3: wave propagation $\mathbf{M} = \mathbf{M}(x_1)\mathbf{M}(x_2) \ldots \mathbf{M}(x_n)$

tunnel junction:



- apply voltage U between left and right regions
- calculate tunnel current I_T
- conductance $G = \frac{I_T}{U} \propto \text{Transmission}$

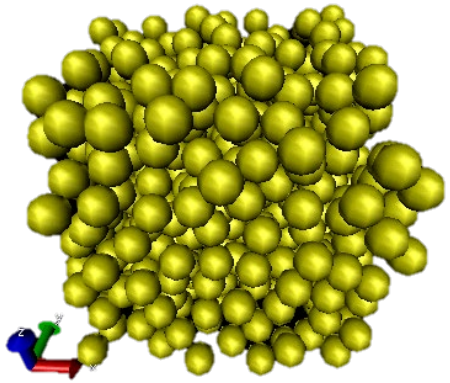
Project 4: molecular dynamics of a simple fluid



atomic motions

molecular dynamics

$$m_i \frac{d^2\mathbf{r}_i}{dt^2} = \mathbf{F}_i$$



fluid