Modelling of metallic nanoalloys at the atomic scale

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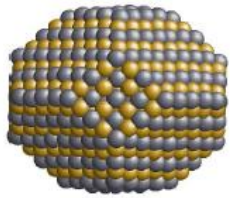

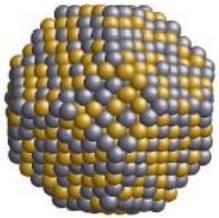

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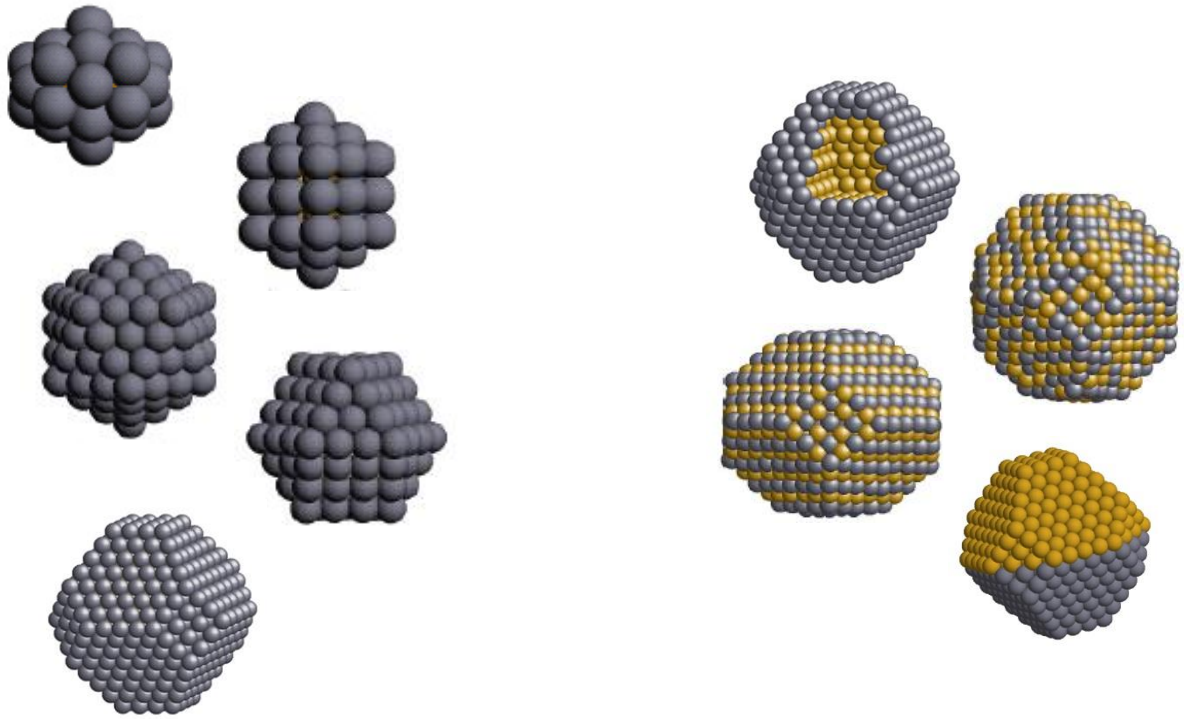
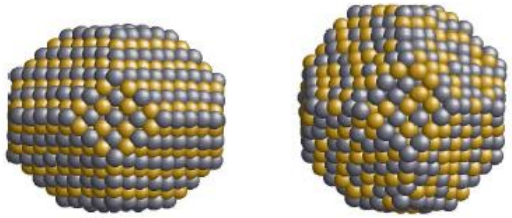
Metallic nanoparticles and nanoalloys

➔ **Properties tightly linked to characteristics : size, shape, composition, surface state**

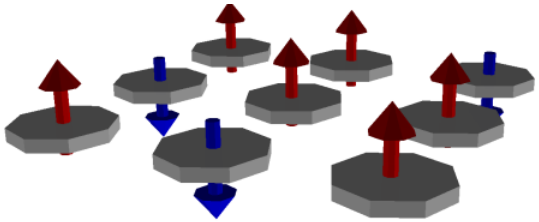


➔ **Wide range of properties and technological applications: optics, magnetism, catalysis, biomedical…**

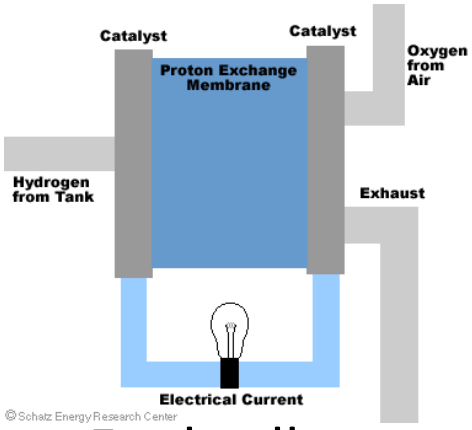
➔ Ordered/disordered nanoalloys



CoPt

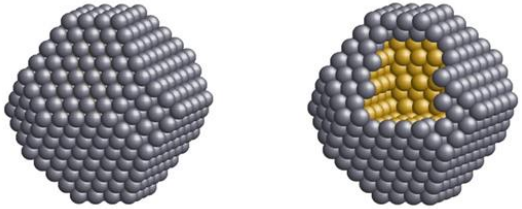


Magnetic storage



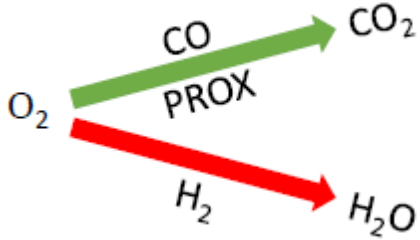
Fuel cells

➔ Core-shell



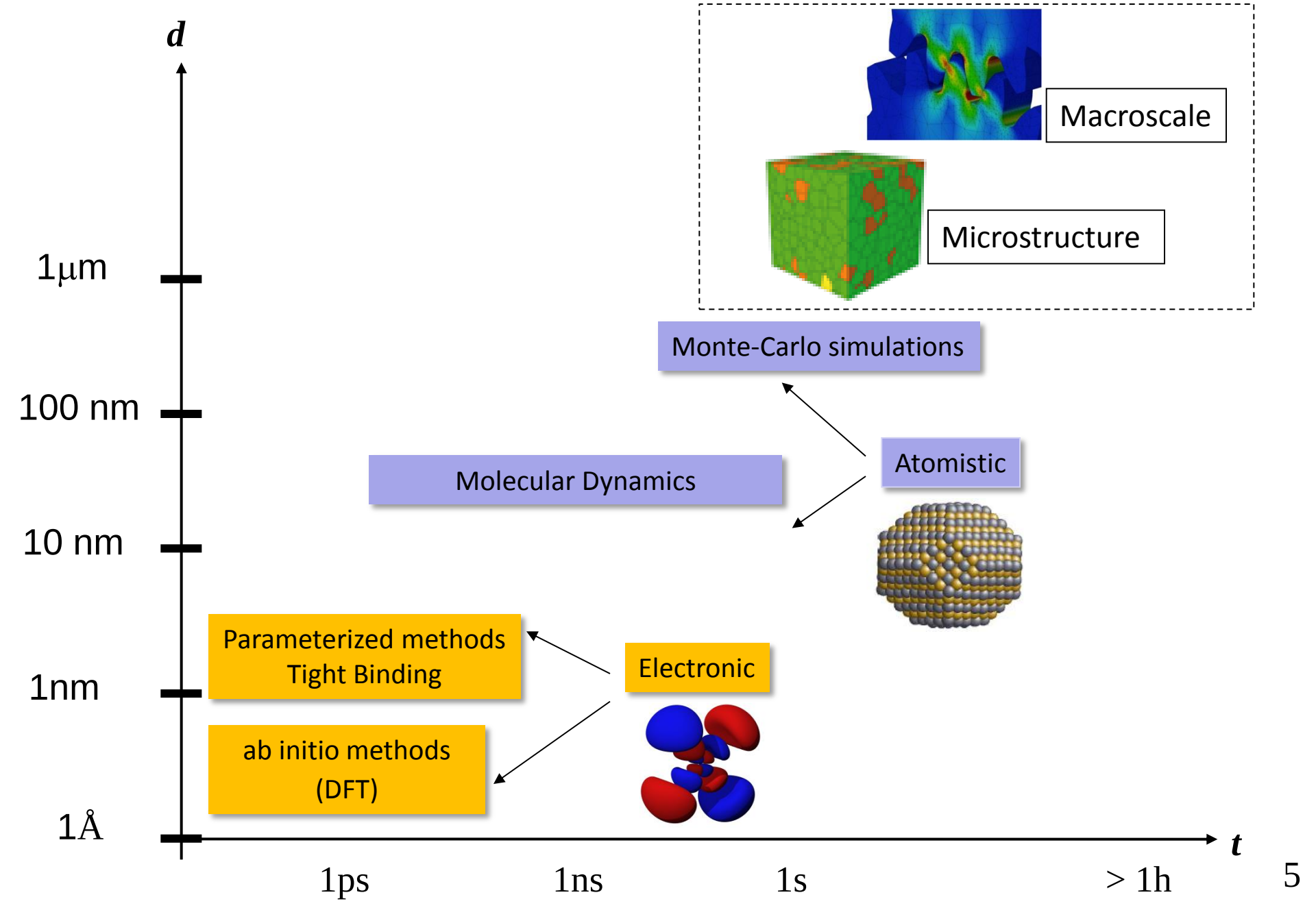
IrPd

Preferential elimination of CO in gaz mixtures



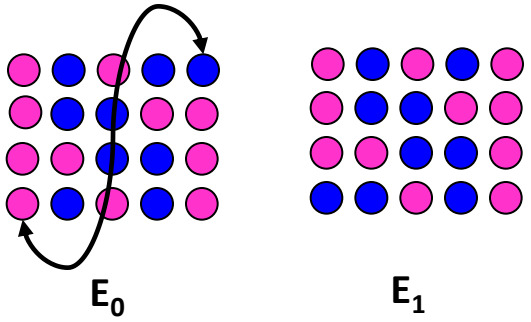
Control of the properties ➔ control of synthesis and structure

Methodology for simulating (nano)materials



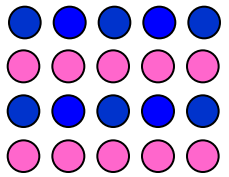
MONTE CARLO simulations

Statistical sampling of the accessible ensemble of configurations



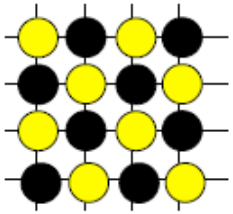
$E_1 < E_0$?

$\exp(-(E_1-E_0)/kT)$

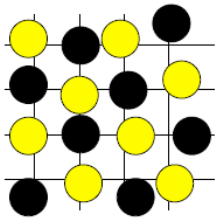


equilibrium

Rigid lattice



With atomic displacements



MONTE CARLO simulations

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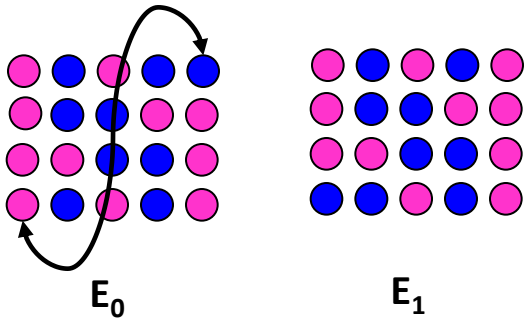

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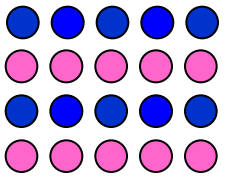
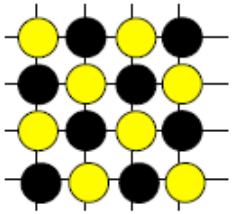


equilibrium

Rigid lattice



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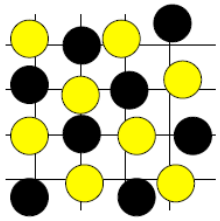

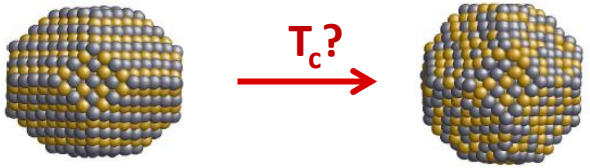

- order/disorder transition : T_C in nanoalloys?
- Analysis: site occupation, order parameter

→ Fortran, matlab, vizualization tools :
rasmol, vmd