09-09-19_AESCM_lesson-01

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1 Electronic structure of solids and surfaces

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1.1 Intro

Electrons in solid state matter is a topic in which physics and chemistry hold different points of view.

Phyicists see the free electrons slightly perturbed by the ion cores. Meanwhile, **chemists** see the valence electrons involved in chemical bonding.

There are four basic types of solids. - Closed shell solids (Ar) - Ionic solids (NaCl) - Covalent solids (diamond) - Metallic solids (Na)

The main thing that sets them apart is the degree of localization of the electrons around the nuclei.

Again, **physicists** and **chemists** have kind of a different set of interests in regards to which properties are interesting to study or calculate.

Physics - Cohesive energy - Relative phase stability - Mechanical properties - Thermal properties - Optical properties - Electronic transport - Magnetism

Chemistry - Structure and bonding - Reactivity - Optical properties

Of course, they also prefer a different set of tools!

Physics - Plane waves & bands - Excitations - Localization - Fermi energy - Reciprocal space - **DFT**

Chemistry - Molecular orbitals - Overlap populations - Electronegativity - Aromaticity - HOMO/LUMO - Point group symmetry - **Hartree Fock method**

Material science is sort of a bridge between physics and chemistry.

It motivates the development of general methods that can properly describe electronic structure in all situations (even molecular solids), bonding, properties, reactivity...

1.2 Use of ab-initio electronic structure methods in material science

- **Clarification/complement** of experimental information by precisely controlling simulation conditions
- **Exploration and prediction** simulating experiments that are difficult (or even impossible) in the lab
- **Design of materials** with cool properties, reducing the *trial and error* loop
- **Paremetrization** of simpler models

1.3 Some examples

1.3.1 Simulation of X-ray diffraction

When you simulate an X-ray diffraction experiment you are actually detecting the distribution of the e density (which implies the position of the e themselves). Nowadays calculating electron density is trivial! (and you need to do it anyway most of the time)

You can also simulate ORTEP drawings (governed by Atomic Displacement Parameters) at different temperatures using electronic structure methods. Neat.

1.3.2 Clarification of ARPES experiments

ARPES means Angle Resolved Photoemission Spectroscopy, and it's used to study the band structure of a solid's occupied levels.

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1.4 Random notes

- A heavy fermion is how a phisicist calls a localized electron
- DFT would work better on heavily compressed systems than in expanded ones

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