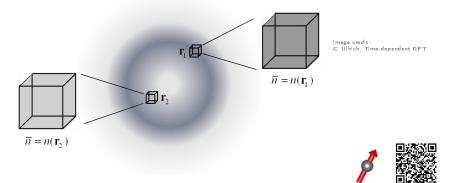
#### En route to electronic correlations



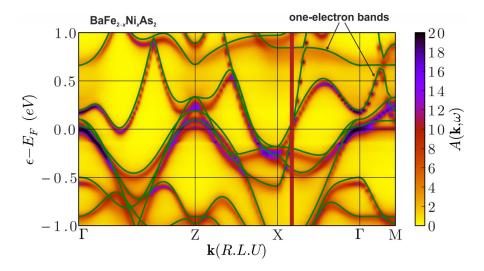
#### density functional theory



by Alexander Tsirlin, Leipzig University

Lecture 14: December 16, 2024

# Crystals with disorder (alloys)



 $A(\mathbf{k},\omega)$  is known as Bloch spectral function

Phys. Rev. B 94, 094512 (2016)

# Hohenberg-Kohn theorem (1964)



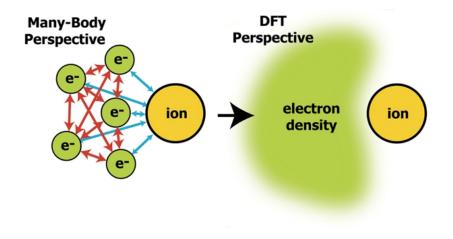
Pierre Hohenberg 1934–2017



Walter Kohn 1923–2016

Nobel prize in chemistry 1998

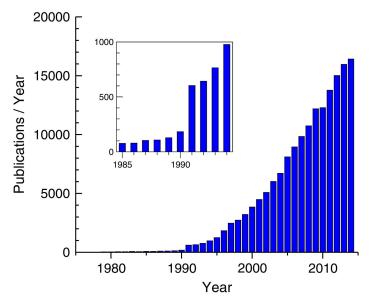
#### Idea of DFT



#### **DFT** = density functional theory

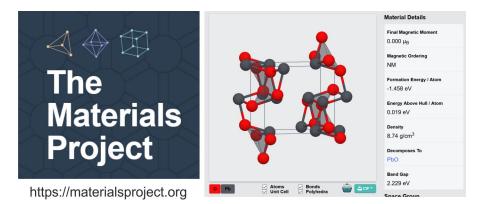
MRS Bulletin 36, 169 (2011)

## Proliferation of DFT



Rev. Mod. Phys. 87, 897 (2015)

### Materials Project



#### Collection of band structures obtained by high-throughput DFT calculations

## Myriad of DFT functionals



J. Chem. Phys. 136, 150901 (2012)

# Jacob's ladder



Image credit: Vladimir Bibikov (fair use)

#### Jacob's ladder

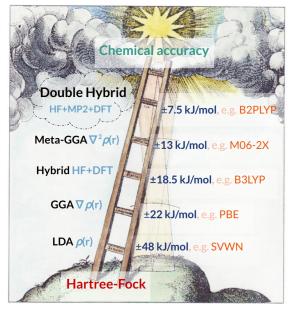


Image credit: Keiran Rowell (fair use)