

# An ab initio study of the hydrogen effect on conductivity of metals

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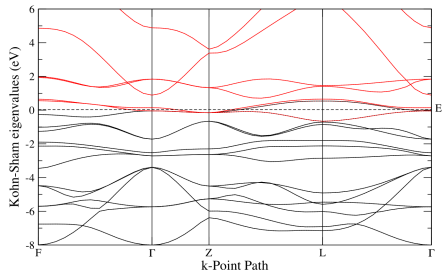
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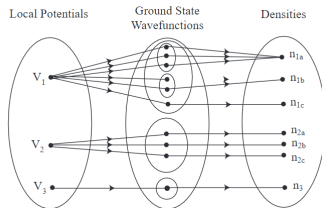
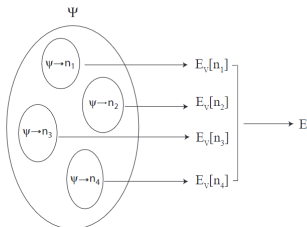
# Computational material science

Objective: How the concentration of Hydrogen effects the electrical conductivity of metals.

- Many-body theory, DFT calculations, no empirical parameters
- Electronic properties



- Find the ground state from the many-body Schrödinger equation
- $\mathbf{H}\psi(\{r_i\}, \{R_I\}) = \mathbf{E}\psi(\{r_i\}, \{R_I\})$
- Born-Oppenheimer approximation,  $m_e \ll M_Z$ ,  $v_e \gg V_Z$
- Define the electron density
- Hartree product,  $\psi(\{r_i\}) = \psi(r_1) * \psi(r_2) * \psi(r_3) * \dots * \psi(r_N)$



## The energy functional

- $E[\{\psi_i\}] = E[\{\psi_i\}] + E_{XC}[\{\psi_i\}]$
- $E_{XC}[\{\psi_i\}]$ , exchange-correlation functional, approximated
- Simplest XC-functionals, LDA, GGA
- Commercial software package, VASP
- Periodic boundary conditions, pseudopotential, plane waves basis set

