Density Functional Theory (DFT) Projects Presentation

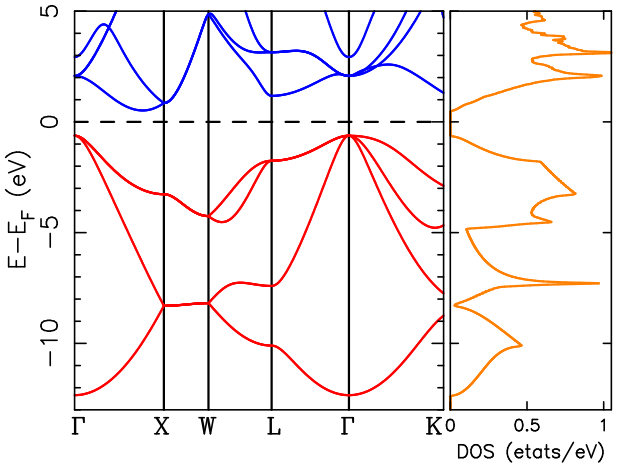
Speaker: Dr. Christophe A. Adessi

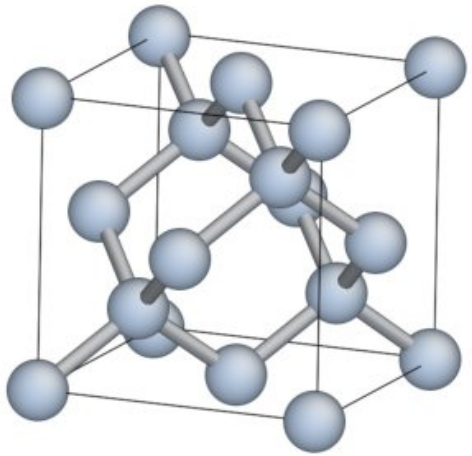
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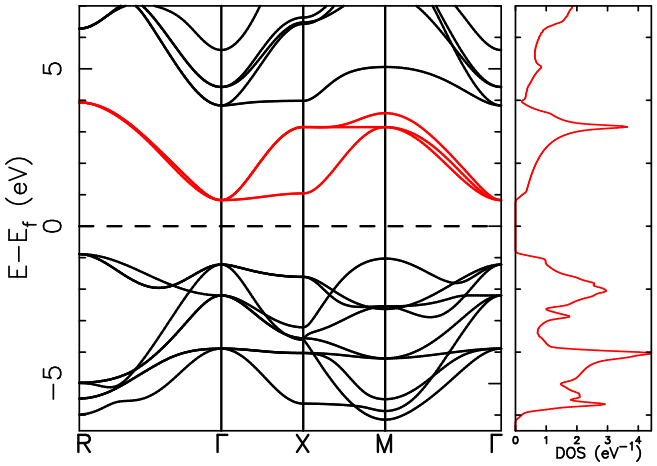
Ge

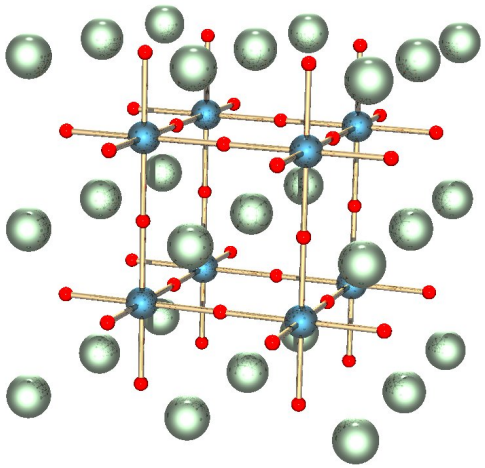




- Semiconducting material
- Band gap issue, influence of XC: LDA *vs* GGA
- n-p Doping (Aluminum / Phosphorus)

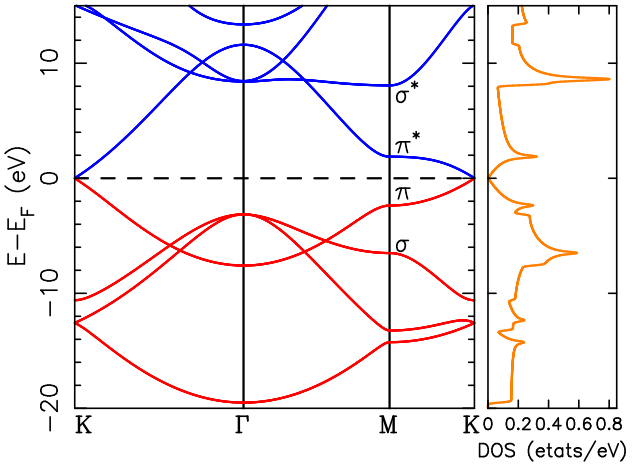
$SrTiO_3$

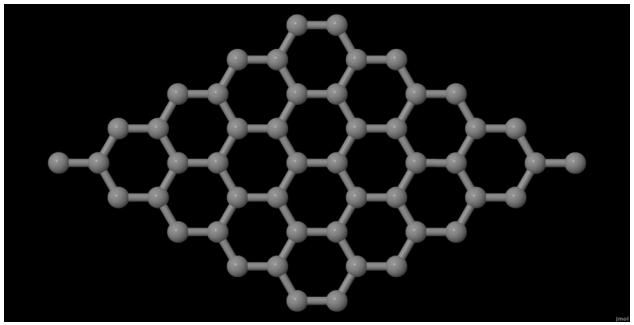




- $SrTiO_3 \Rightarrow$ Perovskites (semiconducting)
- Can be doped (La, V, ..) in substitution
- Dopant may lead to localized (defect) states

Graphene





- Graphene is a Semi-Metal
- Hexagonal 2D structure
- Various type of defects (5×7, Vacancy ...)
- n-doping with adsorbed Alkalis

Expectations

Basic Results

- Define the Optimal Plane Wave cut-off Energy (Total energy as function of $E_{\text{cut-off}}$)
- Define the Optimal # of k-points (Total energy as function of k-points)
- Predict the lattice parameter / Bulk Modulus using the Murnagham eq. of states. Compare results with experimental values.
- Plot the Band stucture and/or the Density of States (DOS). Locate the Fermi Level (Semiconductor or metal?).

Advanced Results

- Influence of defects on electronic properties
- Require a supercell (repetition of the unit cell) and structural optimization (already done for you)
- Study of the influence of dopants (n/p doping):
  - Phosphorus or Al in substitution in Ge
  - La or V in subtitution (to Sr or Ti) in $SrTiO_3$
  - Potassium (alkali) adsorption in Graphene
- Study of the influence of structural defects:
  - 5×7 defect in Graphene
  - C vacancy in graphene
- Influence of the XC functional: (LDA vs GGA) for Ge
- All these calculations will require to plot the DOS and/or the Projected Density of States (PDOS)