Revisiting the electronic structure of ErAs/GaAs(001) interface

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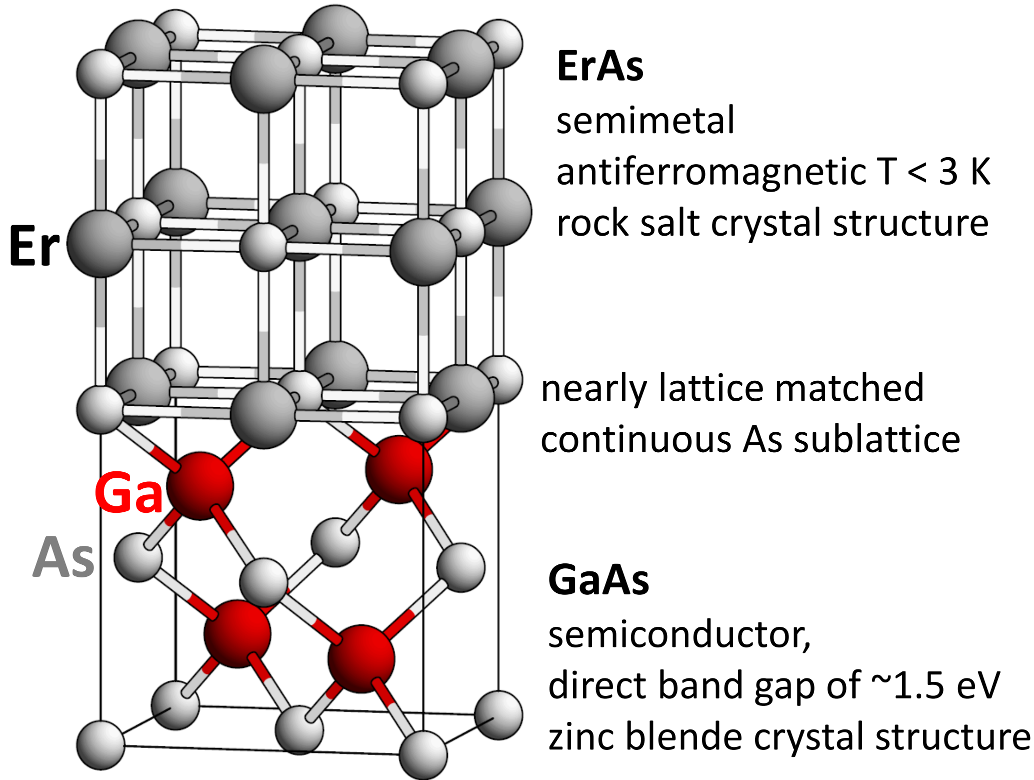
Rare earth pnictides on III-V semiconductors



ErAs
semimetal
antiferromagnetic T < 3 K
rock salt crystal structure

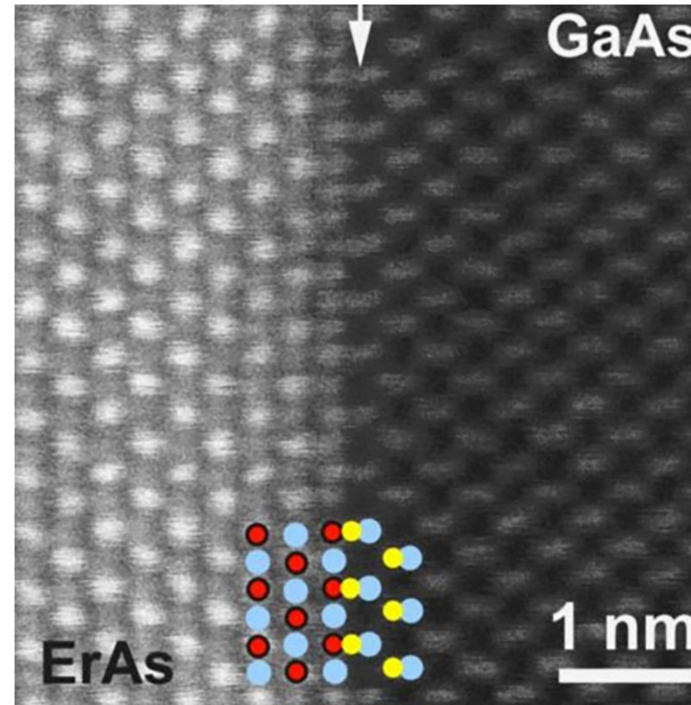
nearly lattice matched
continuous As sublattice

GaAs
semiconductor,
direct band gap of ~1.5 eV
zinc blende crystal structure

Epitaxially lattice matched metal- semiconductor contacts
- Nature and impact of the interface states?
- Will ErAs thin film become a semiconductor in the limit of few monatomic layers?

ErAs/GaAs(001) grown by molecular beam epitaxy (MBE)

C. J. Palmstrom, N. Tabatabaie, and S. J. Allen, Appl. Phys. Lett. **53**, 2608 (1988)



ErAs/GaAs(001):
- **Ga terminated interface**
- **As sublattice continuous**

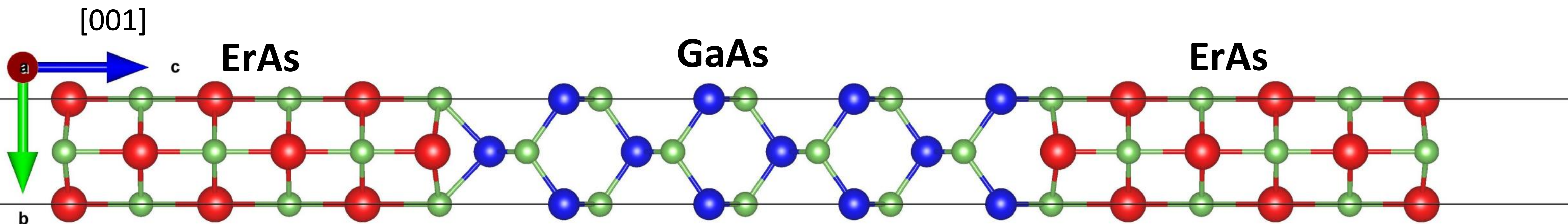
D. O. Klenov *et al.*,
Appl. Phys. Lett. 86, 241901 (2005)

[110]

W. R. L. Lambrecht *et al.*, Solid State Commun. **108**, 361 (1998)
K. T. Delaney *et al.*, Phys. Rev. B **81**, 165312 (2010)

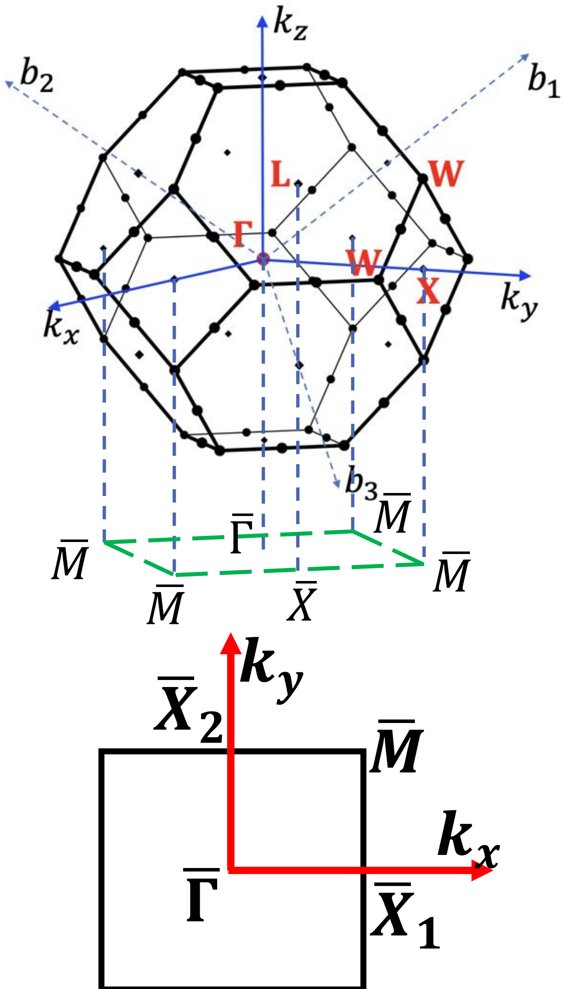
Computational approach

- Density functional theory (DFT) within the generalized gradient approximation
- Tests performed using the HSE06 hybrid functional
- PAW method for electron-ion interaction
- Atomic positions are relaxed until forces are less than 0.01 eV/Å
- VASP code

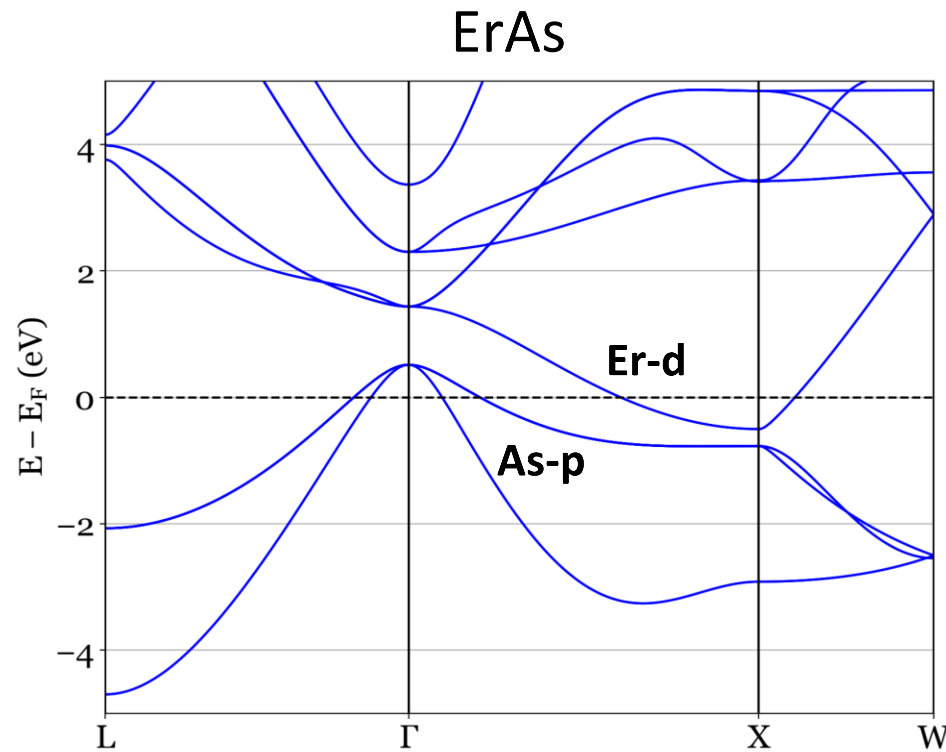


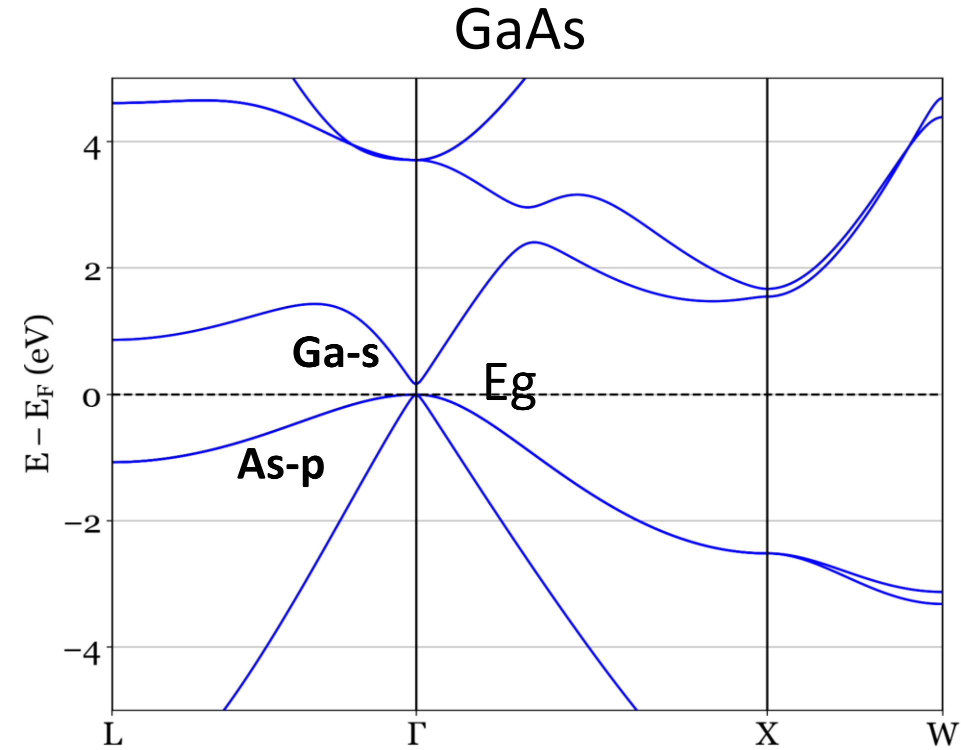
Band structures of ErAs and GaAs at GGA

- ErAs is a semimetalic while GaAs is a semiconductor



(effect of spin-orbit coupling not taken into account)

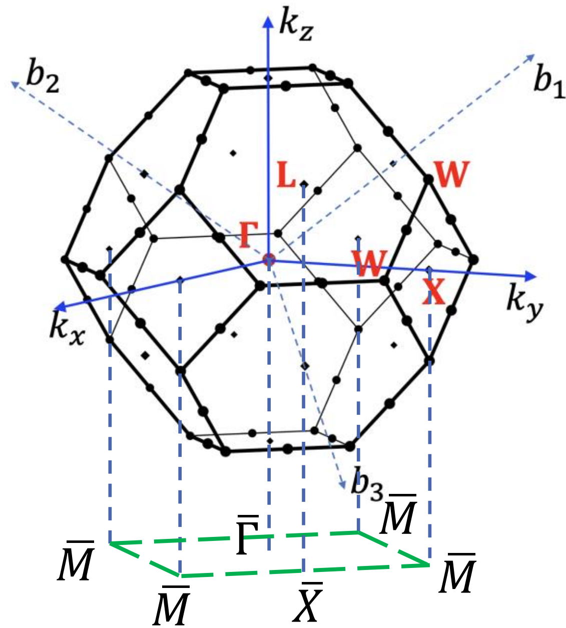


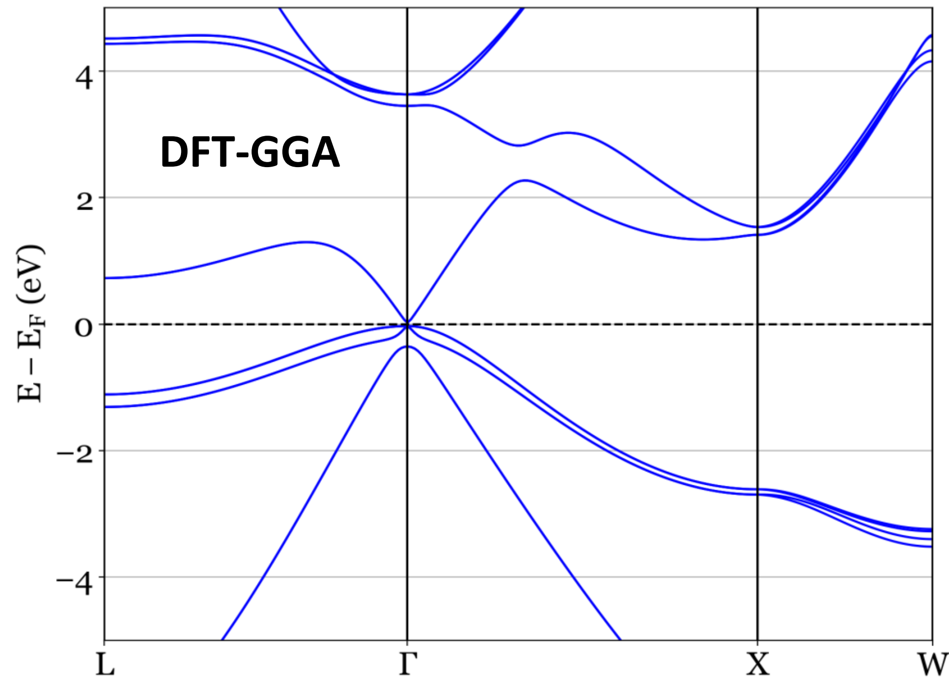


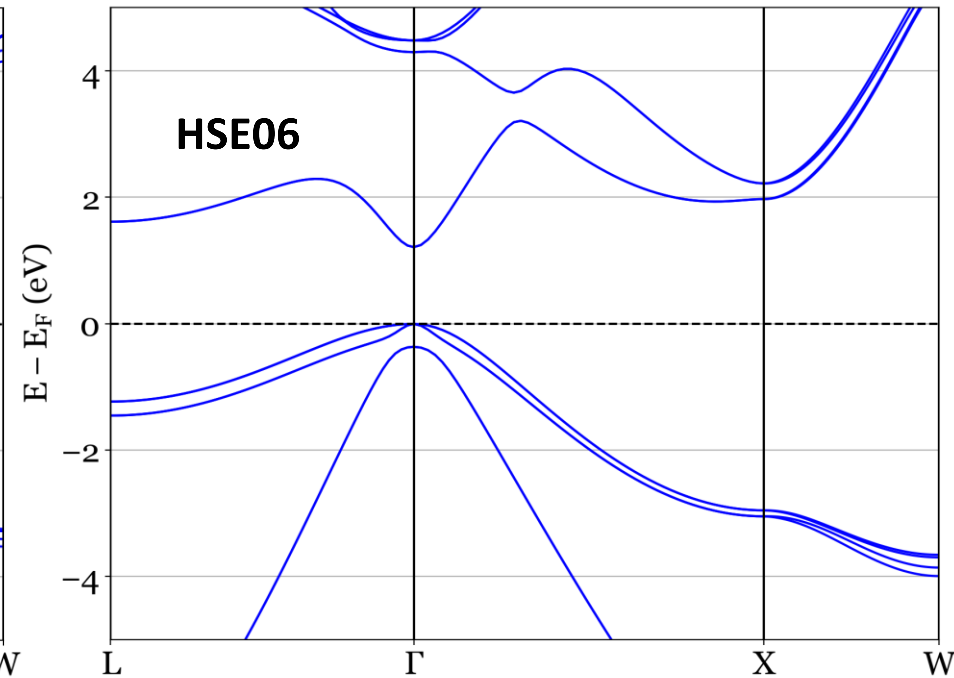
Band gap is underestimated in GGA

Band structure of GaAs including SOC

- Top of the valence band split into 2+1 bands at Γ due to SOC
- Band gap of GaAs at HSE06 is very close to the experimental value

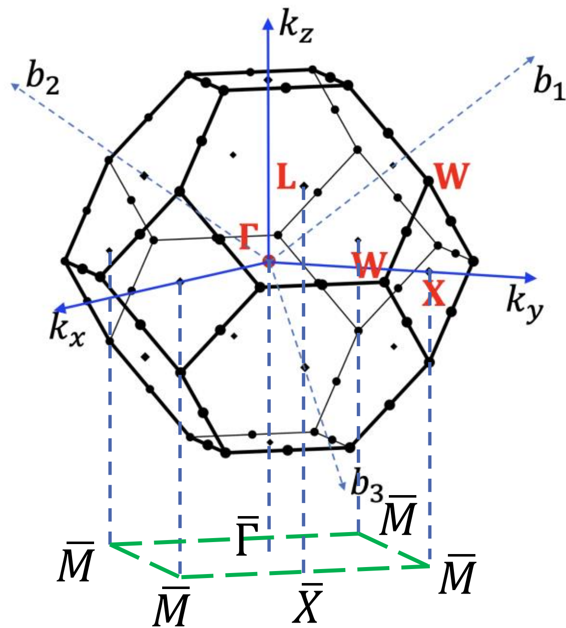


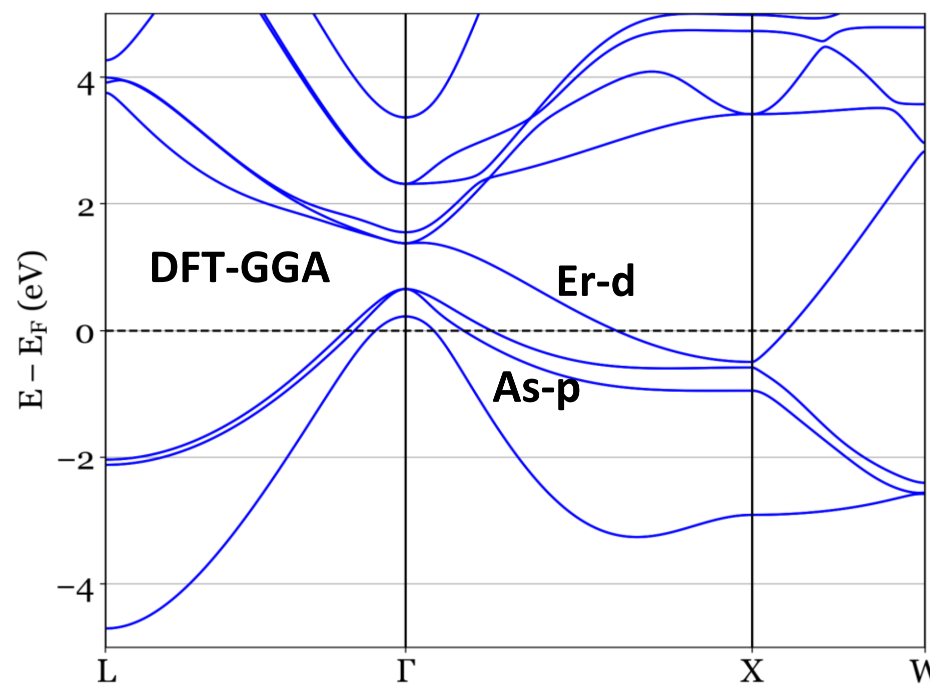


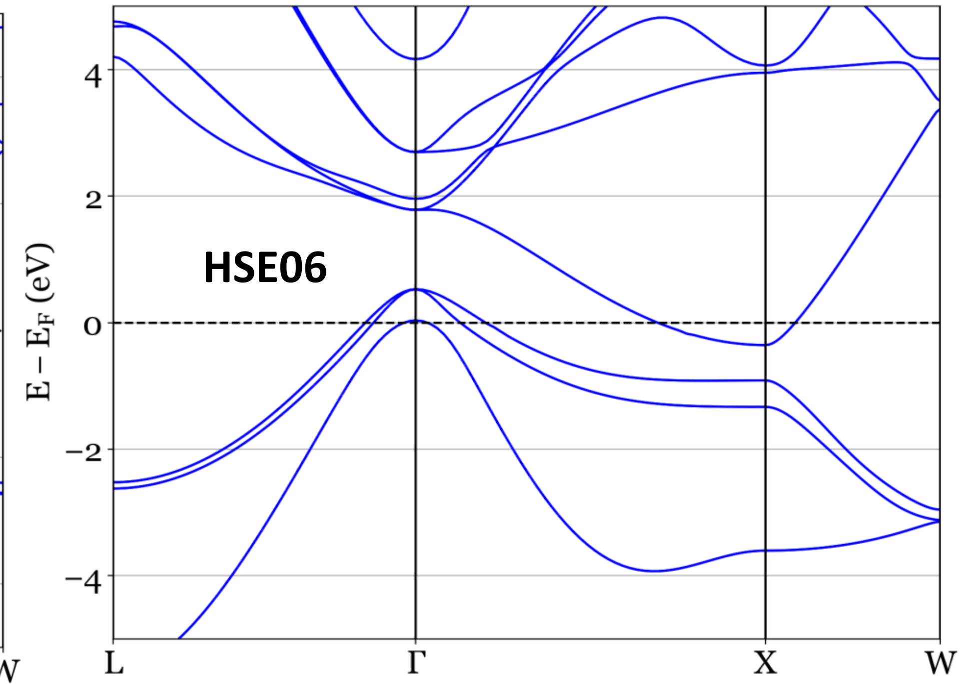


Band structures of ErAs including SOC

- Top of the valence band split into 2+1 bands at Γ due to SOC
- Carrier concentration in HSE06 is in good agreement with experimental value







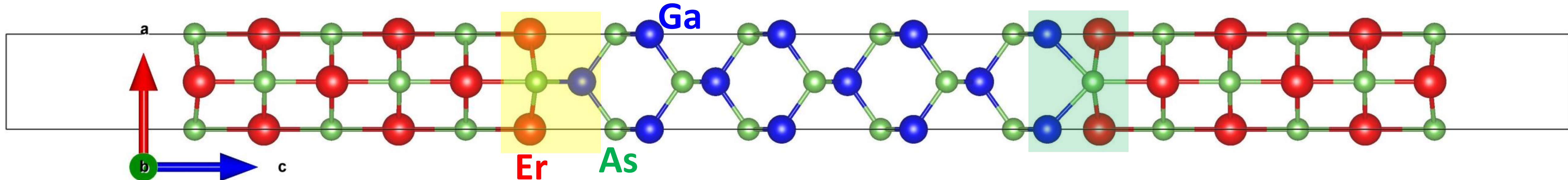
Top of the hole pockets split into 2+1
Hole bands also split at X
Er-d band is not degenerate at X

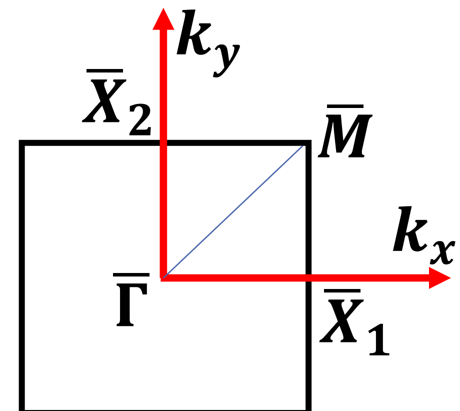
Concentration	DFT-GGA	HSE06	Exp.
$n\ (10^{20}\mathrm{cm}^{-3})$	5.56	3.3	1.8 – 4.69

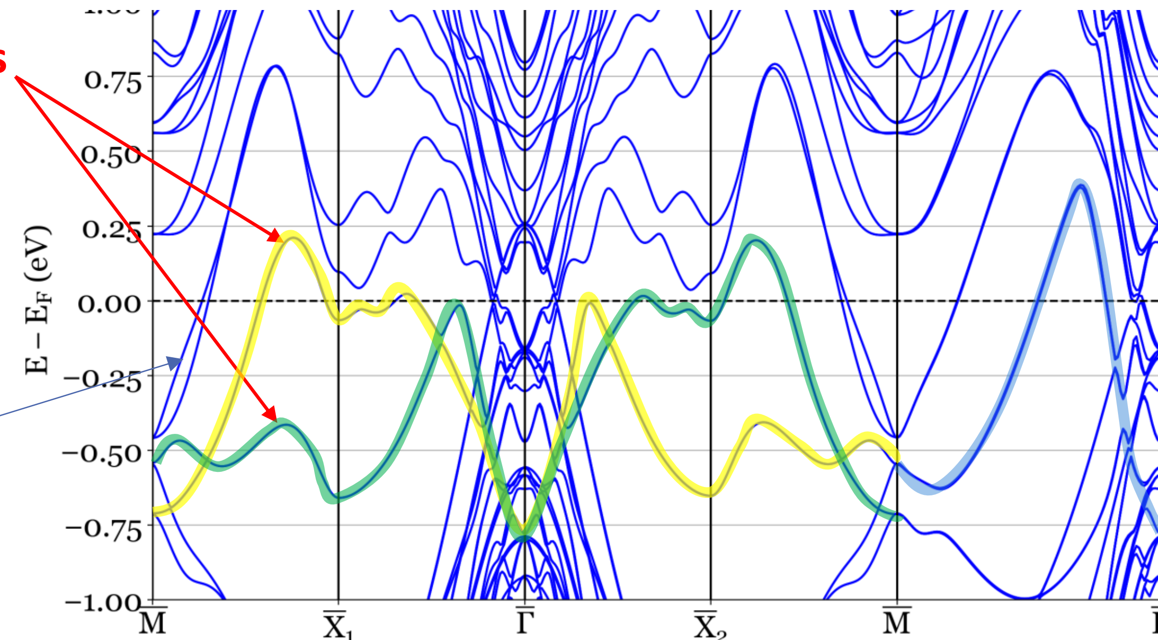
Khalid et al., PHYSICAL REVIEW B **101**, 125105 (2020)

ErAs/GaAs(001) band structure

- Structure of the interface with Ga-termination, continuous As-sublattice between the two materials
- One interface state for each state, E_F pinned by interface states







- ✓ DFT-GGA functional
- ✓ Fixed in-plane lattice parameter to that of GaAs
- ✓ All atoms are allowed to relax

Band structure projected on interface atoms

Band structure projected on interface atoms

As33
Ga13
As37
Er7

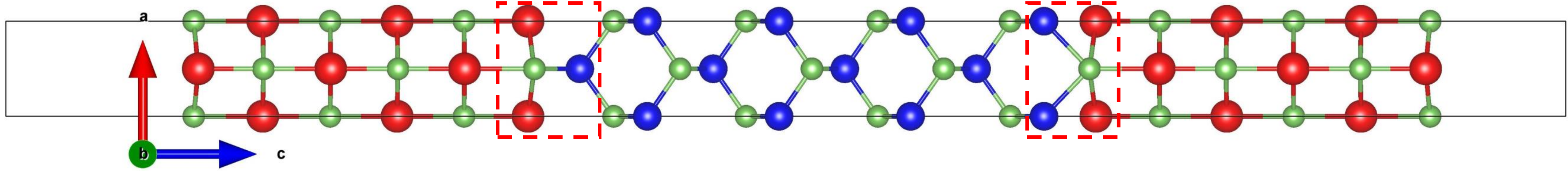
Er7
Ga13
As37
As33

$E - E_F$ (eV)

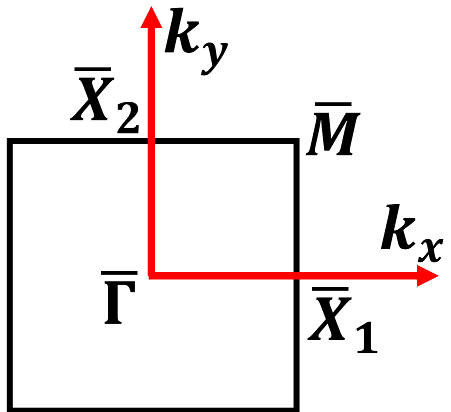
$\bar{M}$ $\bar{X}_1$ $\bar{\Gamma}$ $\bar{X}_2$ $\bar{M}$ $\bar{\Gamma}$

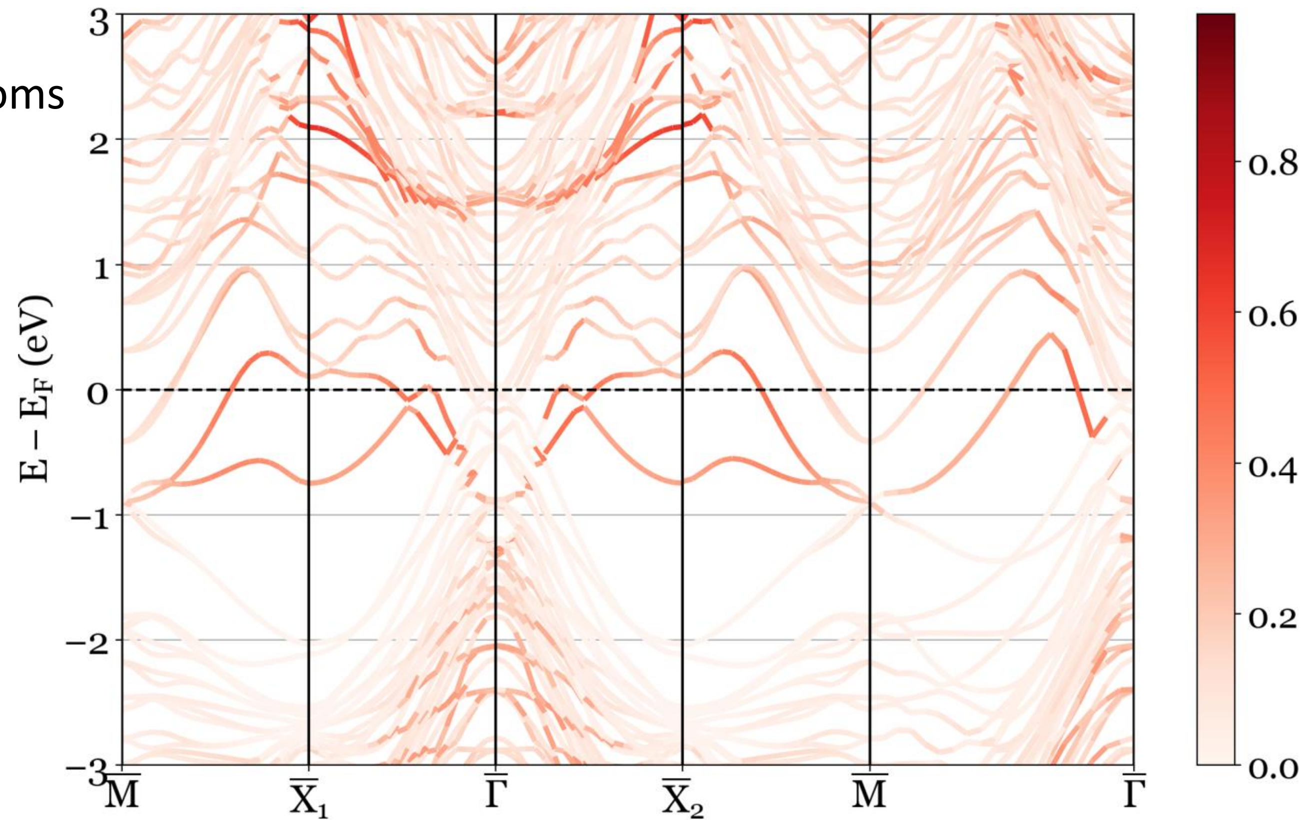
$|\langle Y^{\alpha}_{lm}|\phi_{n\mathbf{k}}\rangle|^2$

ErAs/GaAs(001) band structure HSE06

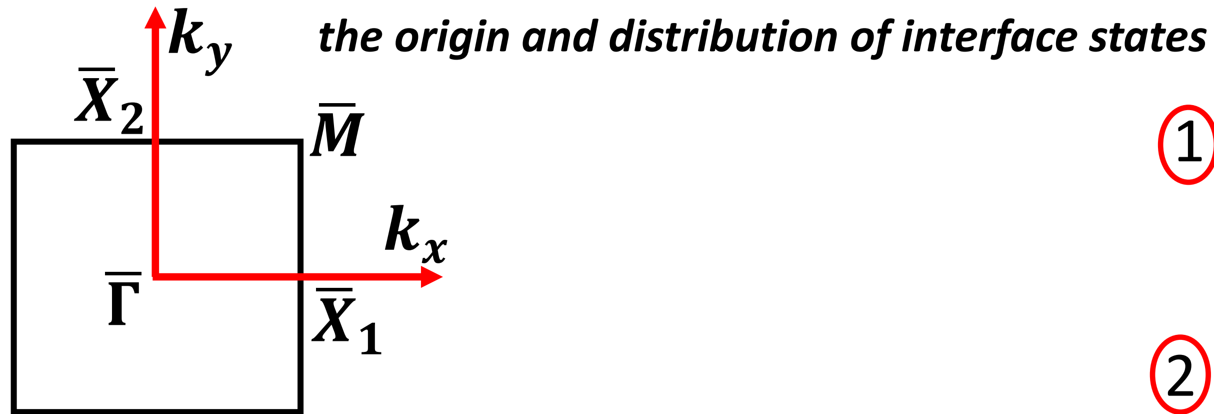


Band projection on interface atoms

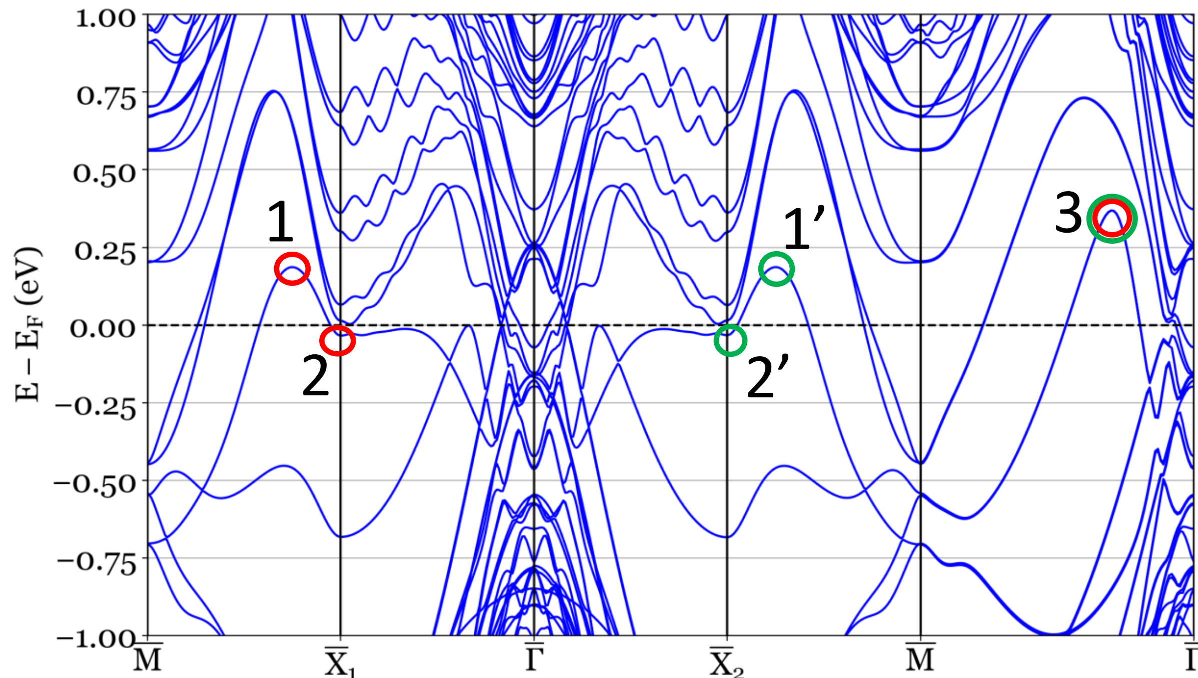


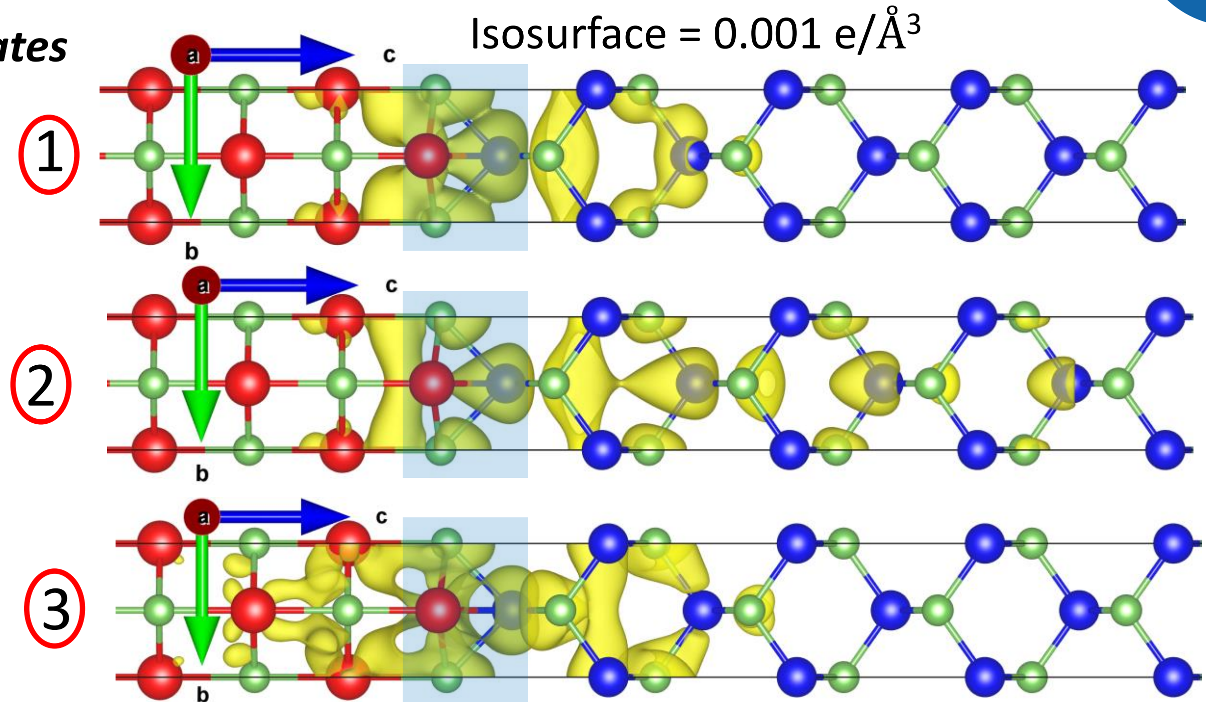


Partial charge density of ErAs/GaAs(001)



the origin and distribution of interface states





- ✓ interface states is highly localized close to the interface region, yet completely delocalized in the plane of the interface.
- ✓ Since the interface state is partially filled, it represents a conducting interface channel (2D hole/electron gas) that is tightly confined to the interface.

Summary

- The existence of interface states in GaAs/ErAs(001) heterostructure
- Fermi level pinning by the interface states
- GaAs/ErAs(001) leads to a partially filled interface bands
  - Completely delocalized in the plane
  - Tightly bound to the interface (within a few ML)
  - 2D hole gas with high hole concentration
  - Metallic interface states persist down to a very thin limit of ErAs film thickness.