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Radiation Damage and Point Defects in GaSb and InAs

Austin Shipley[1],

Dr. Peter A. Schultz[2], Dr. Evan M. Anderson[2], and Dr. Boris Kiefer[1].

1: Department of Physics
New Mexico State University

2: Sandia National Laboratories

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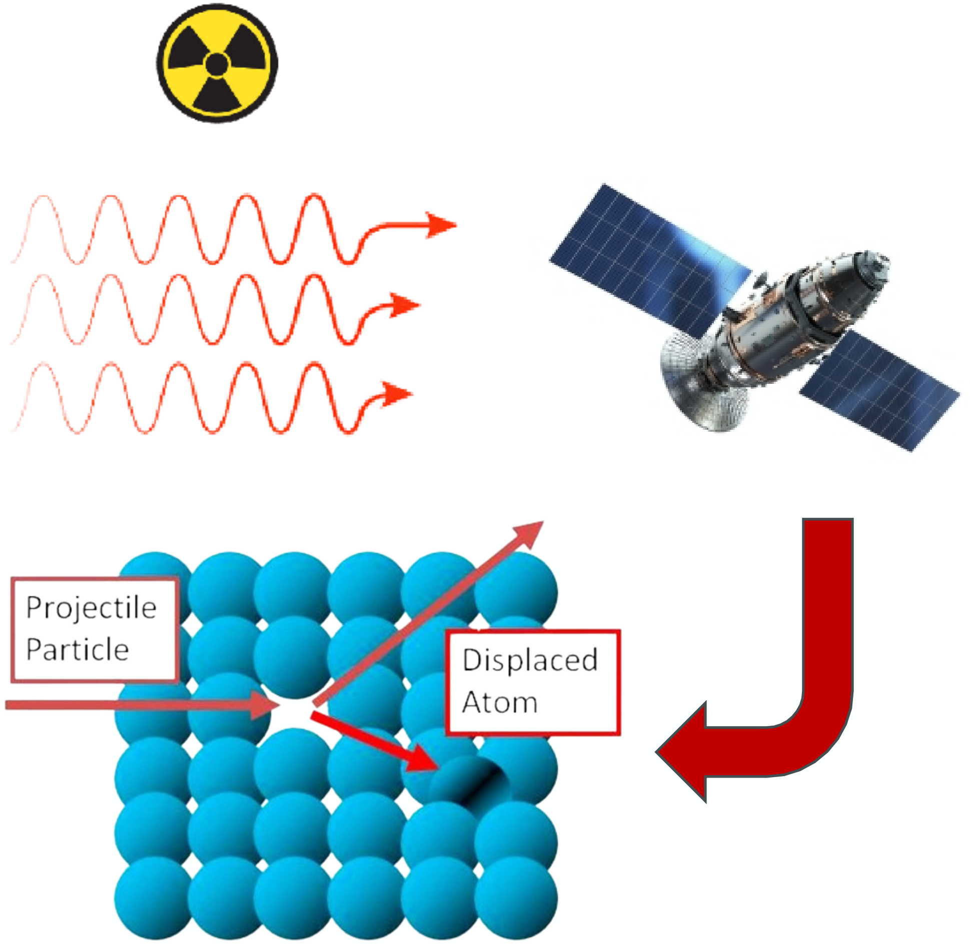
Introduction & Motivation

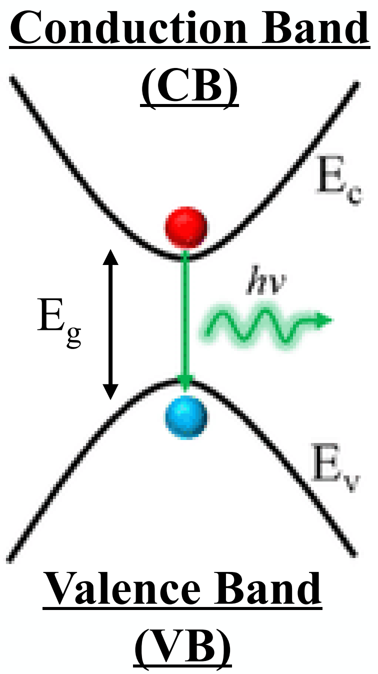


- **Infrared (IR) sensors**, optoelectronics, thermophotovoltaics, satellite solar cells
- **Narrow band gap** semiconductors ($E_g \leq$ **1.1 eV**) are an attractive class of materials (e.g., GaSb, InSb, InAs…)
- Challenge: Radiation-induced **defect** states
  - ➢ Affects IR device **performance**
  - ➢ Creates **alternative** electronic pathways for electronic relaxation
- Impacts: Device **failure** and **false** signal readings

https://wpo-altertechnology.com/wp-content/uploads/2015/12/Displacement-damage.jpg

Recombination

Pristine Crystal, Defect free



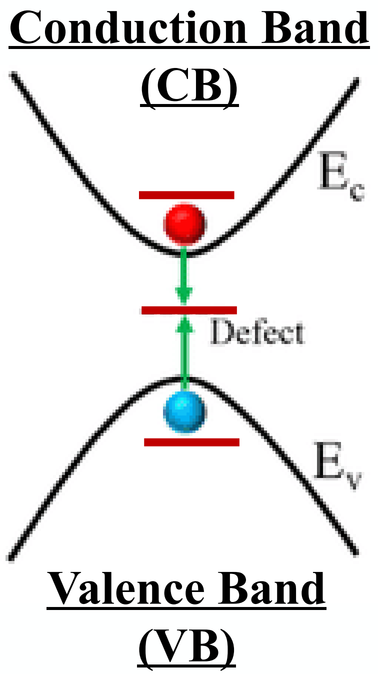
Radiative Recombination

- **CB** electron **recombines** with **VB** hole
  - ➢ Accompanied by the release of a **photon**
- Involves **spontaneous emission**, **absorption/gain**, and **stimulated emission**
- **Important** for high-performance **IR sensors**

Non-Radiative Recombination

- Electronic states in bandgap trap **electrons** and/or **holes**
  - ➢ Accompanied by the release of a **phonon** (heat)
- Bandgap states **adversely** affect IR device **performance** and **reliability**

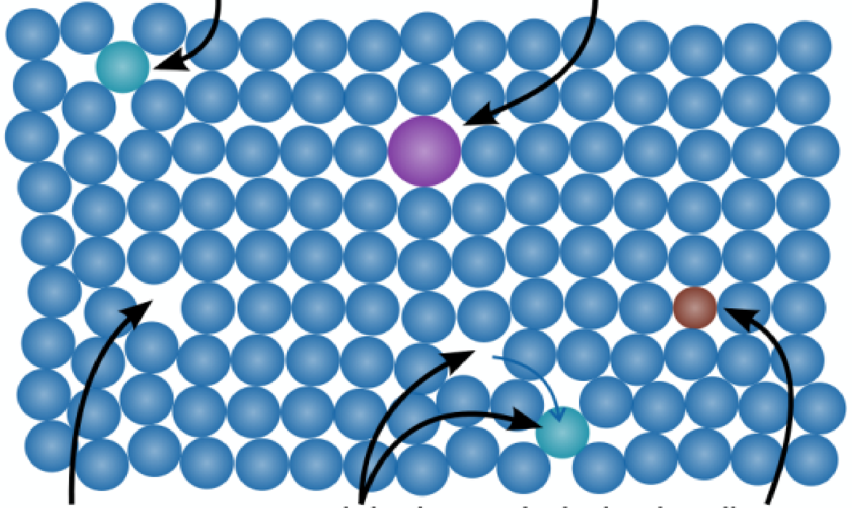
Defect-induced electronic relaxation pathway



Recombination states within the bandgap are important loss-mechanisms in semiconductor materials

https://www.researchgate.net/figure/Effects-associated-with-defects-in-semiconductors-A-Radiative-recombination-pathway-of_fig1_346766691

Point Defects



- Point defects are **localized imperfections** in an otherwise perfectly periodic crystalline lattice
  - ➢ Changes **bonding**
  - ➢ New **electronic states** may occur in the **bandgap**

Classifications

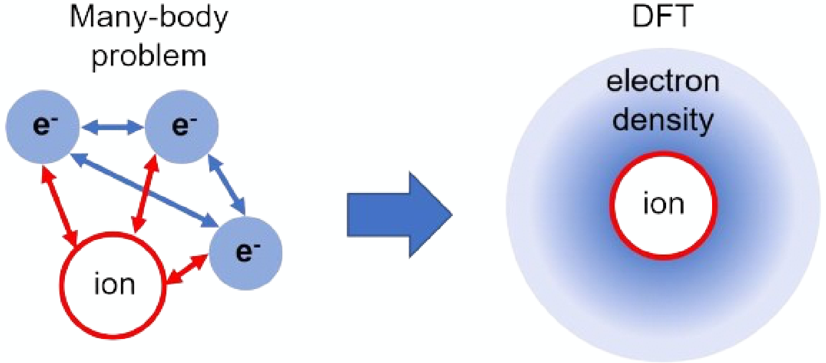
- **Vacancy**: Missing atom from a lattice site
- **Antisite**: **Substitutional** defect where a group V atom occupies group III site (and vice versa)
  - i.e. Electron Level 2 (**EL2**): Sb_{Ga}
    - **Metastable** defect state of GaSb
- **Interstitial**: Atom occupies crystalline void
- **Frenkel Pair**: Interstitial-vacancy pairs

Objective: Build workflow to evaluate point defects in narrow-gap semiconductors

https://www.researchgate.net/figure/Effects-associated-with-defects-in-semiconductors-A-Radiative-recombination-pathway-of_fig1_346766691

Approach

Density Functional Theory (DFT)



Hohenberg-Kohn Theorems

➔ Kohn-Sham Equations

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \underbrace{V(\mathbf{r})}_{\text{e}^- \text{ and nuclei interactions}} + \underbrace{V_H(\mathbf{r})}_{\text{Hartree potential}} + \underbrace{V_{XC}(\mathbf{r})}_{\text{Exchange-correlation}}\right]\psi_i(\mathbf{r}) = \epsilon_i\psi_i(\mathbf{r})$$

Kohn, Sham (1964)

e- and nuclei interactions — *Hartree potential* — *Exchange-correlation*

Challenges

- **Exchange-correlation** universal but unknown
- Computationally **inexpensive** DFT methods (i.e. LDA, GGA) **underestimate** the bandgap
  - ➢ Improved by **hybrid functionals** (i.e. HSE06, PBE0) and/or **GW**, but more computationally **expensive**.

Approach

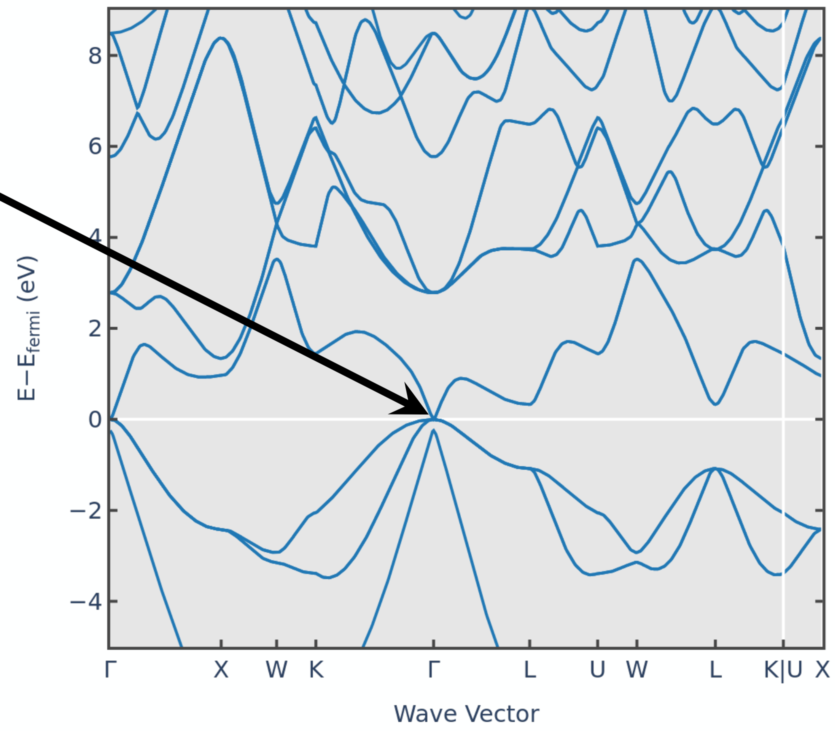
- **Observation**:
  - Standard DFT (i.e. LDA, GGA) exhibits **metallic** properties in experimentally verified **small band gap** materials (i.e. GaSb, InAs,…)

Solution: expand standard DFT approach

- Improve bonding description
- **Hubbard+U+V** method *(Lee and Son, 2020)*

Solid	GGA (eV)	ACBN0 (eV)	Hubbard+U+V (eV)	HSE (eV)	GW (eV)	Expt. (eV)
GaAs (B3)	0.55	0.68	1.28	1.11	1.85	1.52
InAs (B3)	0.00	0.00	0.46	0.57	0.31	0.42

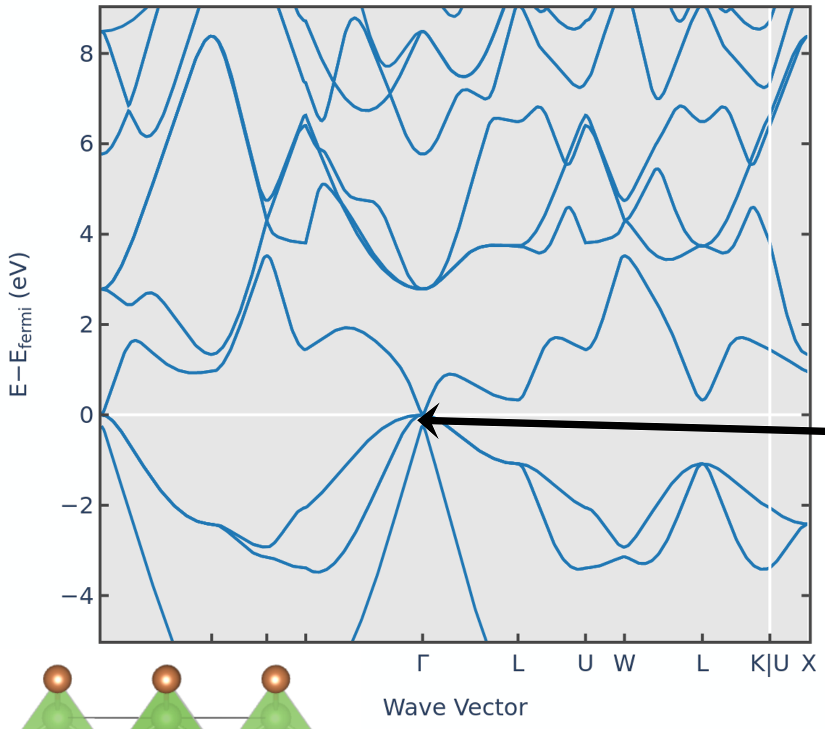
GaSb

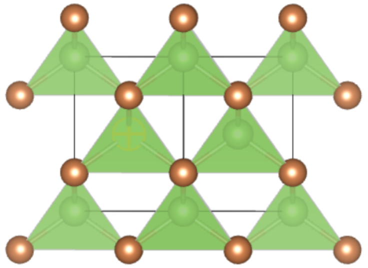


Materials Project, **mp-1156**

Addressing the Band Gap Problem

Materials Project: GaSb (*mp-1156*)



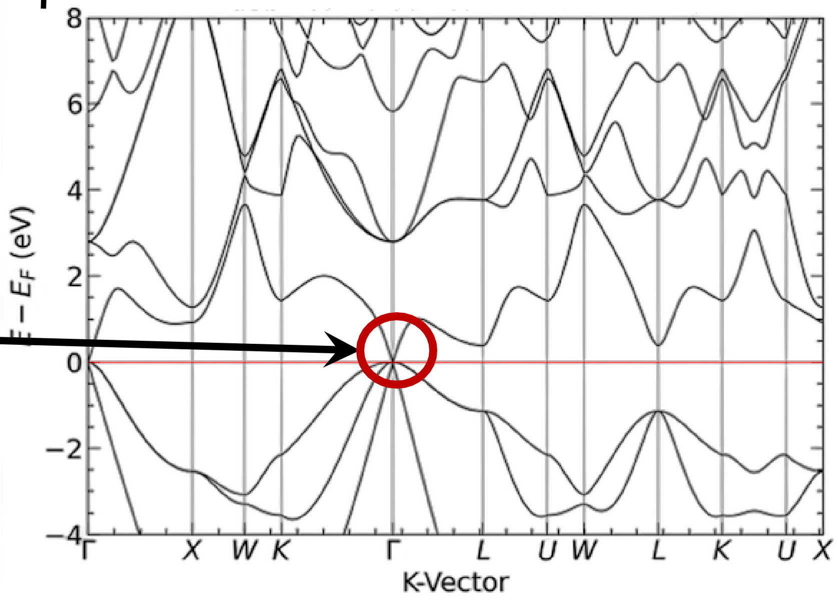


Exp. E_g (T = 0K): 0.813 eV

(Wu & Chen, 1992)

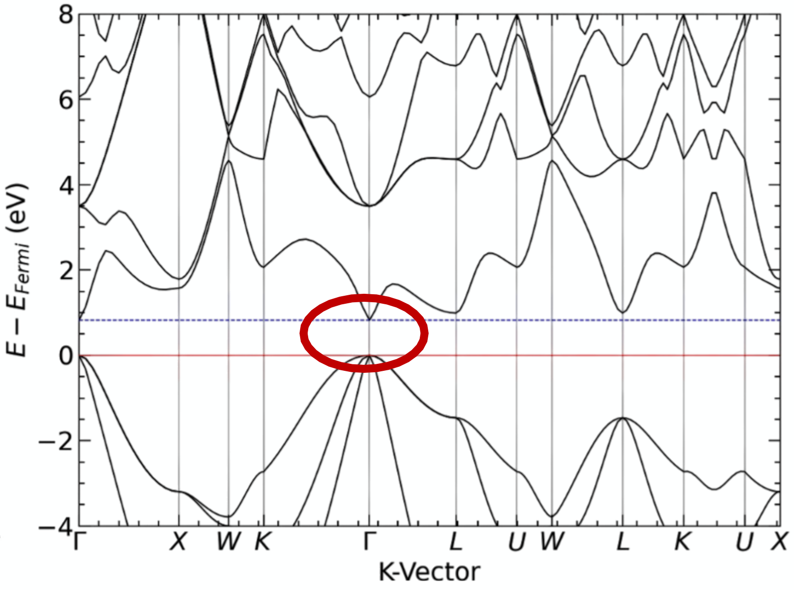
GaSb

DFT: 2 Atom Cell



- **E_g = 0 eV**
  - ➢ **Metallic**

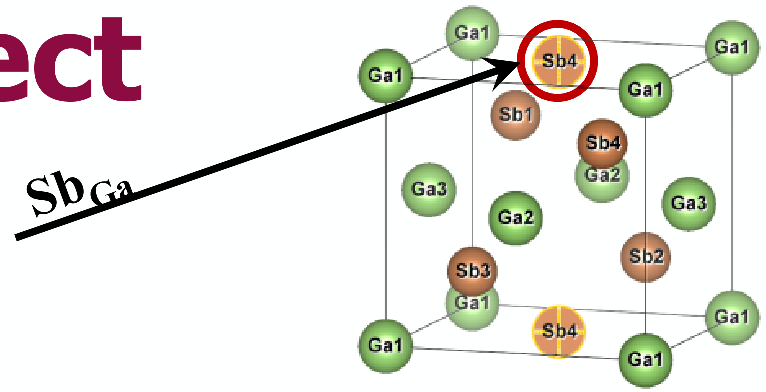
Hubbard+U+V: 2 Atom Cell



- **E_g = 0.81 eV**

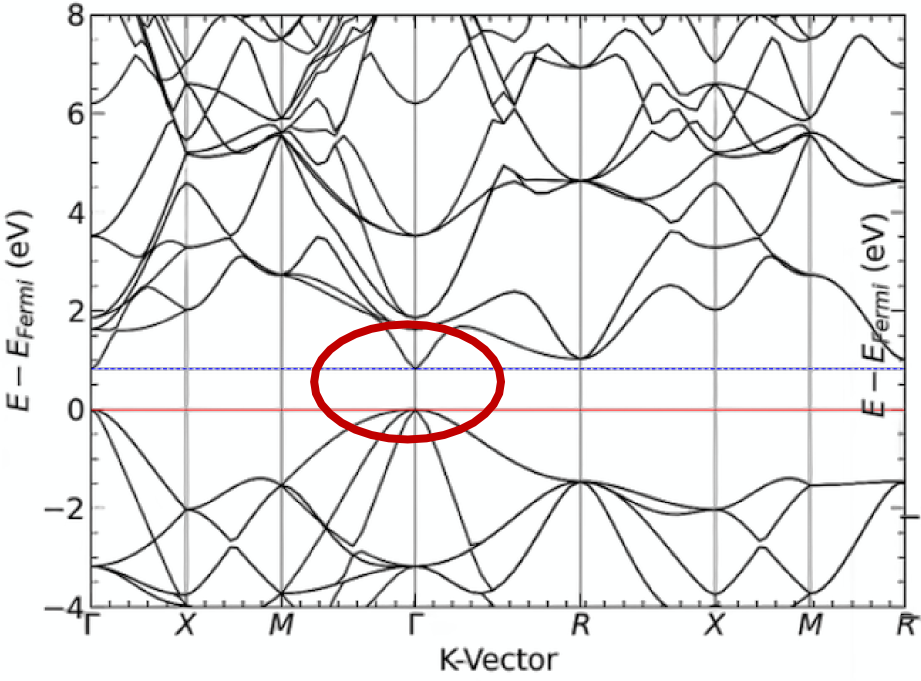
Hubbard U+V opens bandgap comparable to experiment

8-atom Antisite Defect (GaSb)



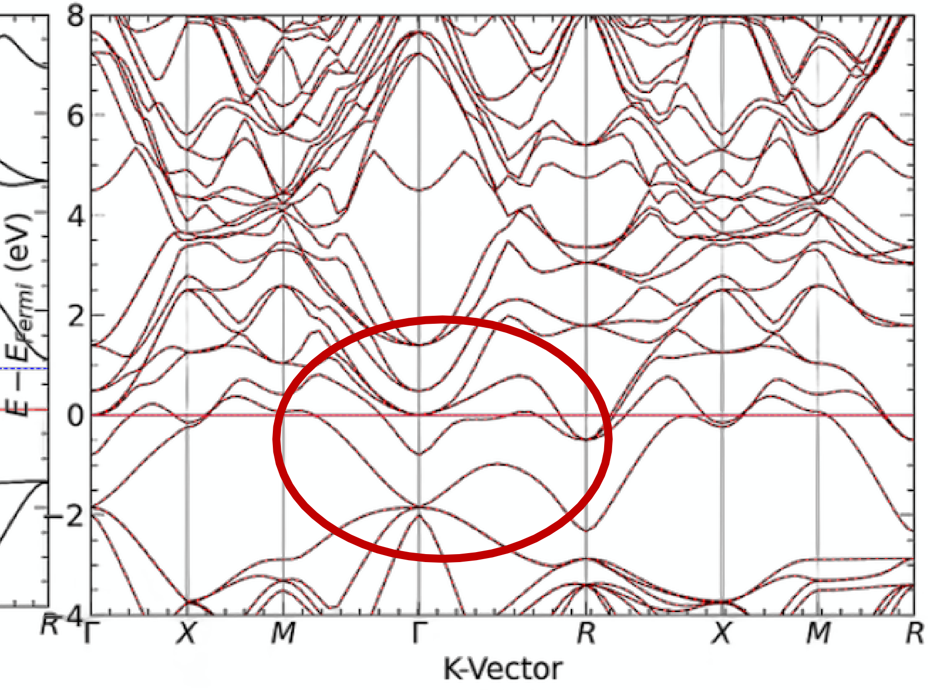
Sb_{Ga}

Pristine (Ga_4Sb_4)



- **E_g = 0.82 eV**

Sb_{Ga} Antisite (Ga_3Sb_5)

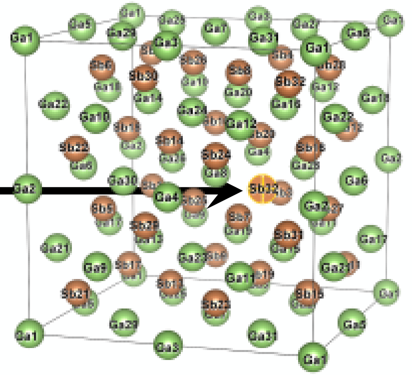


- **Metallic**
  - ➢ E_g = **0 eV**
- Non-magnetic
- Defect-induced **dispersion** larger than **bandgap**.
- Occurrence of **recombination center** unclear
- Need **larger unit cell(s)**

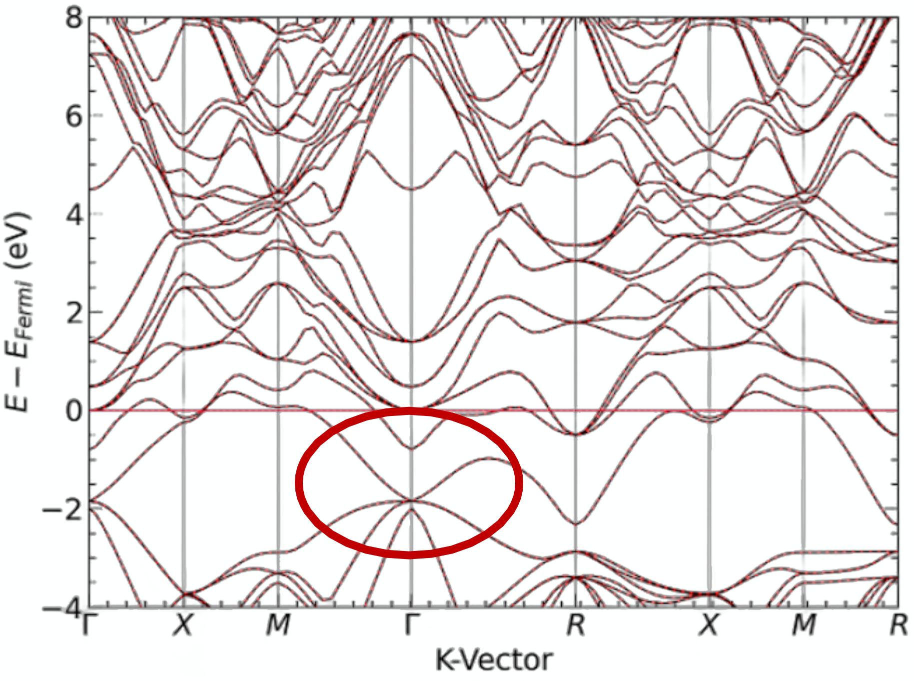
64-atom Antisite Defect (GaSb)

Sb_{Ga}

Sb_{Ga}

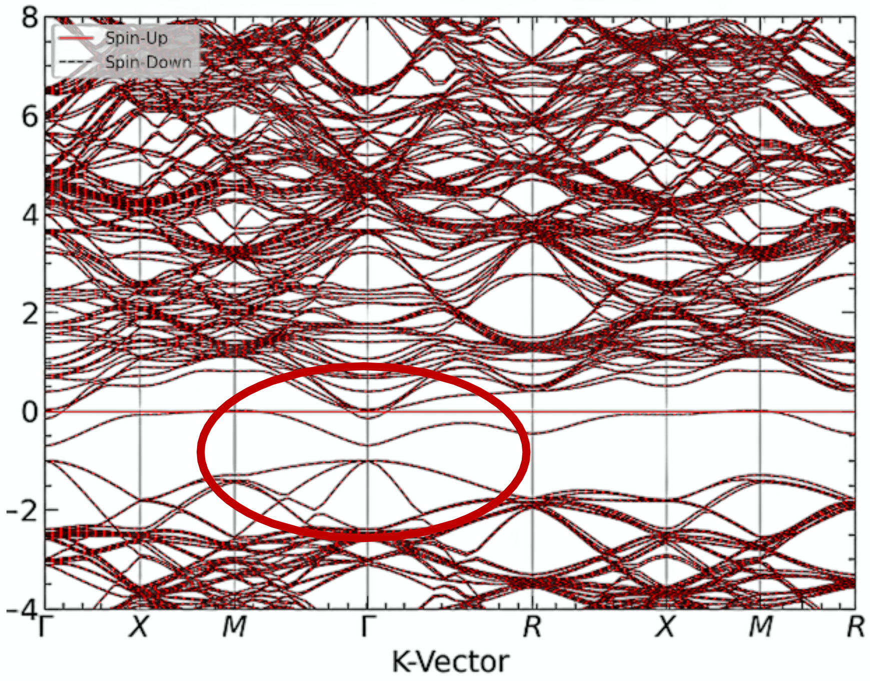


Sb_{Ga} Antisite (EL2) (Ga_3Sb_5)



8-atoms

Sb_{Ga} Antisite (EL2) ($Ga_{31}Sb_{33}$)



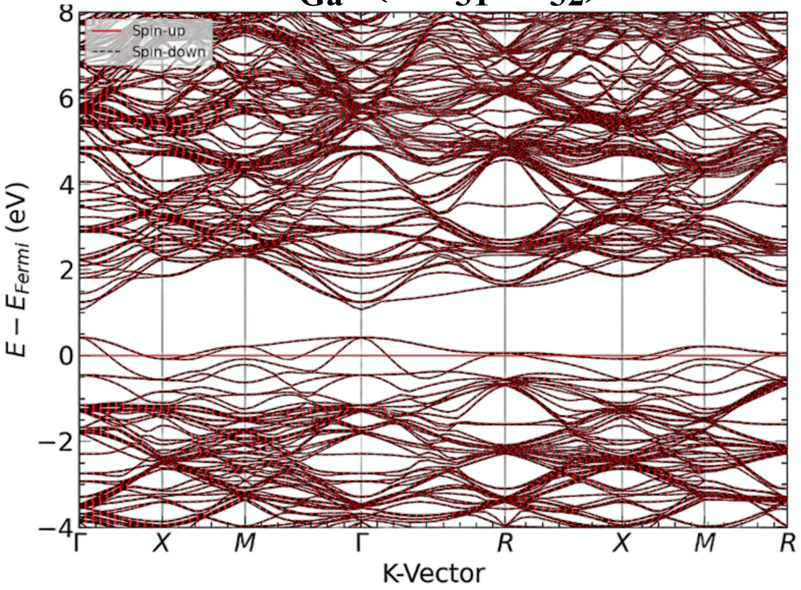
64-atoms

- **Metallic**
  - E_g = **0 eV**
- Defect band **0.3 eV** above **VBM**
- Formation of defect-induced **recombination center**
- Sb_{Ga} Antisite: **Defect likely forms recombination center**

64-atom Vacancy Defects (GaSb)

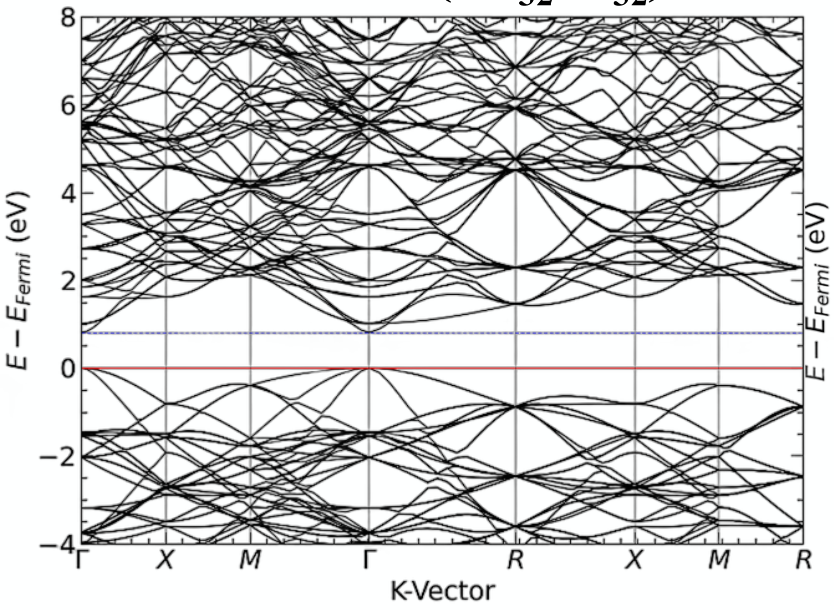
V_{Ga} V_{Sb}

V_{Ga}: $(Ga_{31}Sb_{32})$



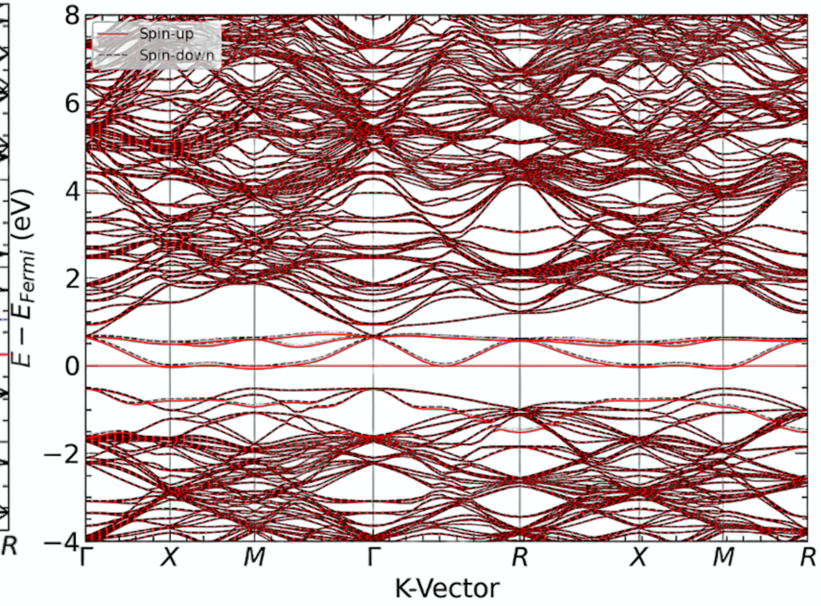
- Metallic
  - ➢ $E_g = 0$ eV
- Electronic defect states not in bandgap
  - ➢ No recombination center

Pristine $(Ga_{32}Sb_{32})$



- Semiconducting
  - ➢ $E_g = 0.82$ eV

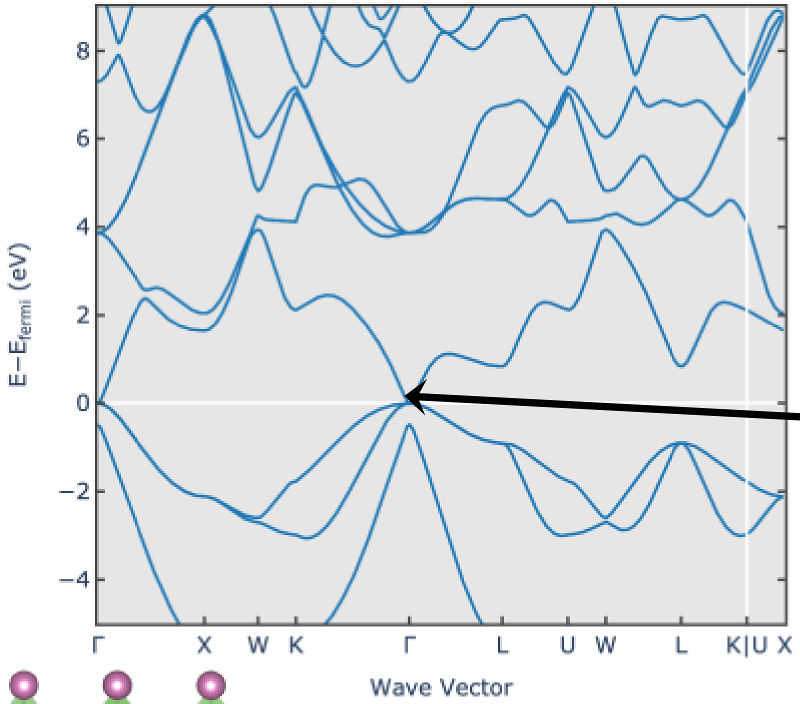
V_{Sb}: $(Ga_{32}Sb_{31})$

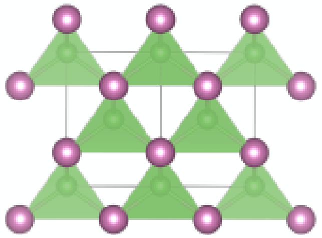


- Metallic
  - ➢ $E_g = 0$ eV
- Electronic defect states in bandgap
  - ➢ Recombination center

InAs & Hubbard+U+V

Materials Project: InAs (*mp-20305*)

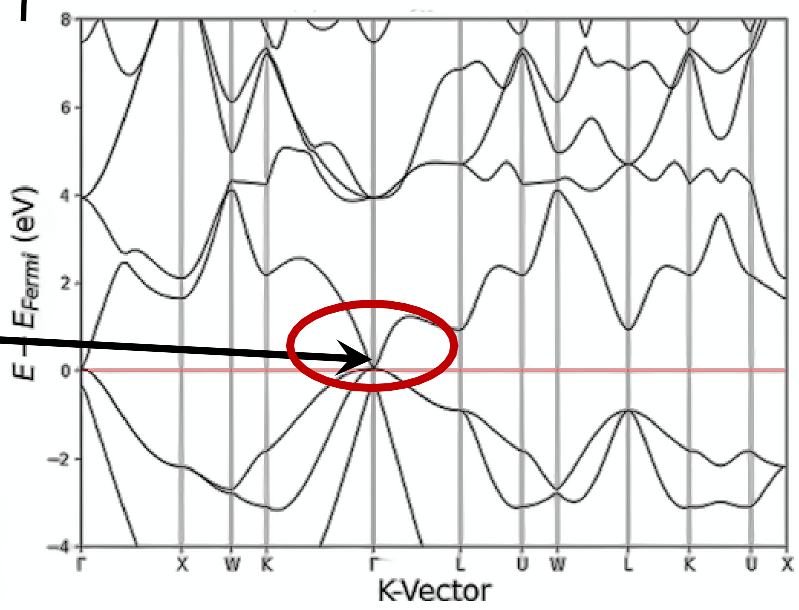




Exp. E_g (T = 0K): 0.42 eV
(*Fang et al. [1990]*)

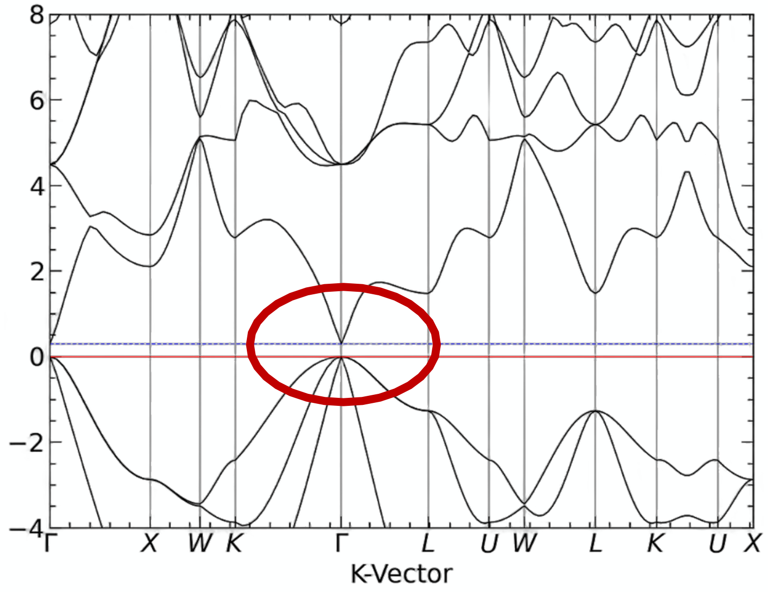
InAs

DFT: 2 Atom Cell



- E_g = 0 eV
  - ➢ **Metallic**

Hubbard+U+V: 2 Atom Cell



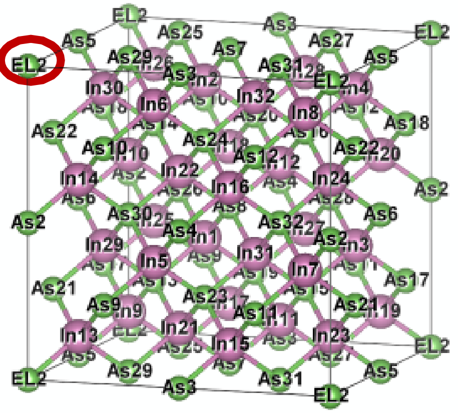
- E_g = 0.30 eV

Hubbard U+V opens bandgap comparable to experiment

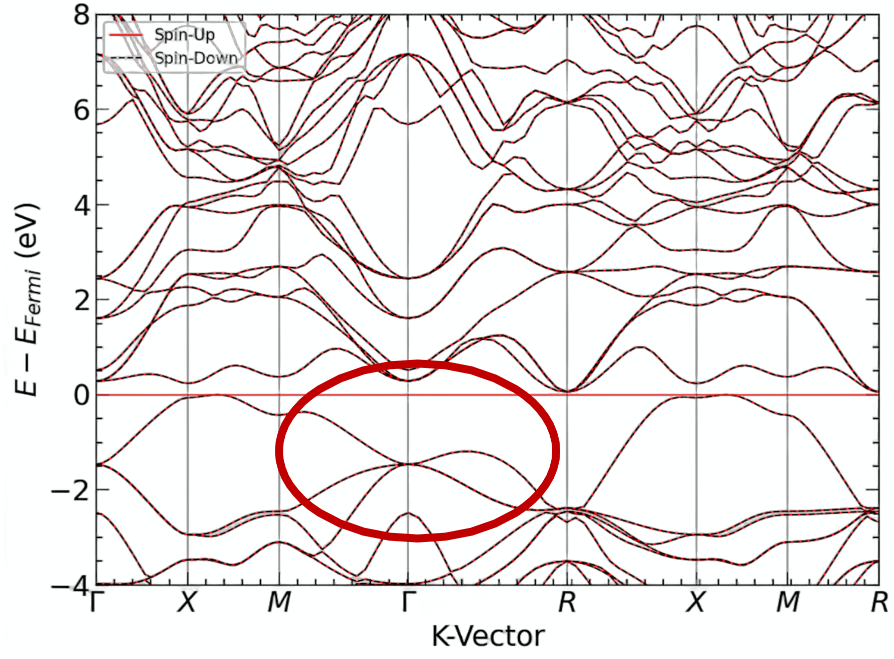
64-atom Antisite Defect (InAs)

As_{In}

As_{In}

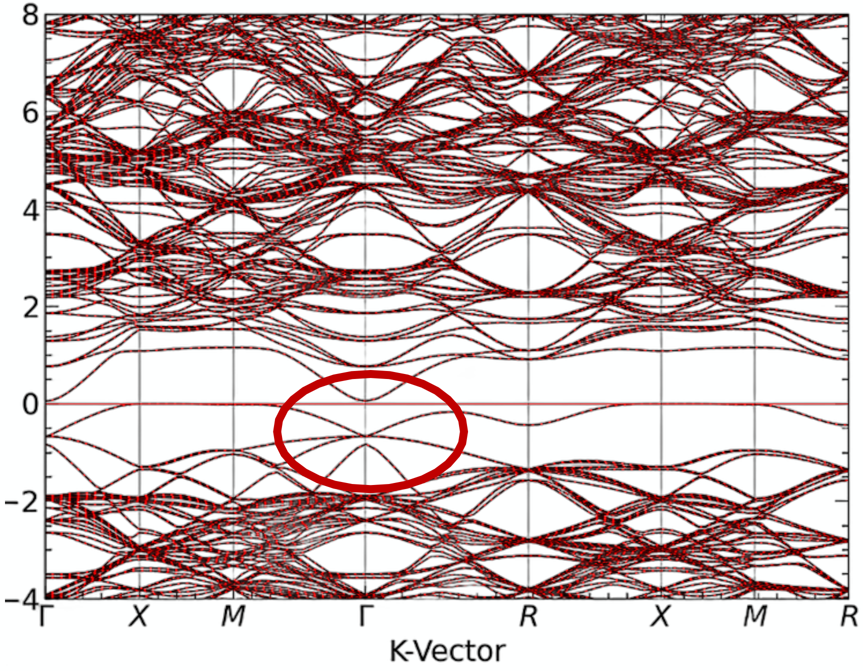


As_{In} Antisite (EL2) (In_3As_5)



8-atoms

As_{In} (EL2)Antisite ($In_{31}As_{33}$)



64-atoms

- **Metallic**
  - ➢ E_g = **0 eV**
- Non-magnetic
- **Electronic defect state appears in the bandgap**
  - ➢ **Recombination center similar to GaSb**

Summary

- Small simulation cells:
  - ➢ Significant dispersion, due to defect-defect interactions
  - ➢ Cannot unambiguously conclude if defects form recombination centers

- Larger simulation cells:
  - ➢ Dispersion decreases
  - ➢ Antisite: Sb_{Ga} & As_{In} → **form recombination centers**
  - ➢ Vacancy: V_{Sb} → **form recombination center**
  - ➢ Vacancy: V_{Ga} → no recombination center

- Defects in GaSb and InAs appear to **behave similarly**

- **Recombination center formation depends on geometry and chemical nature of the defect**
  - ➢ **Need a detailed library of defect/electronic structure relationships to evaluate the performance impact of defects in narrow bandgap semiconductors.**

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