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Radiation Damage and Point Defects in InSb

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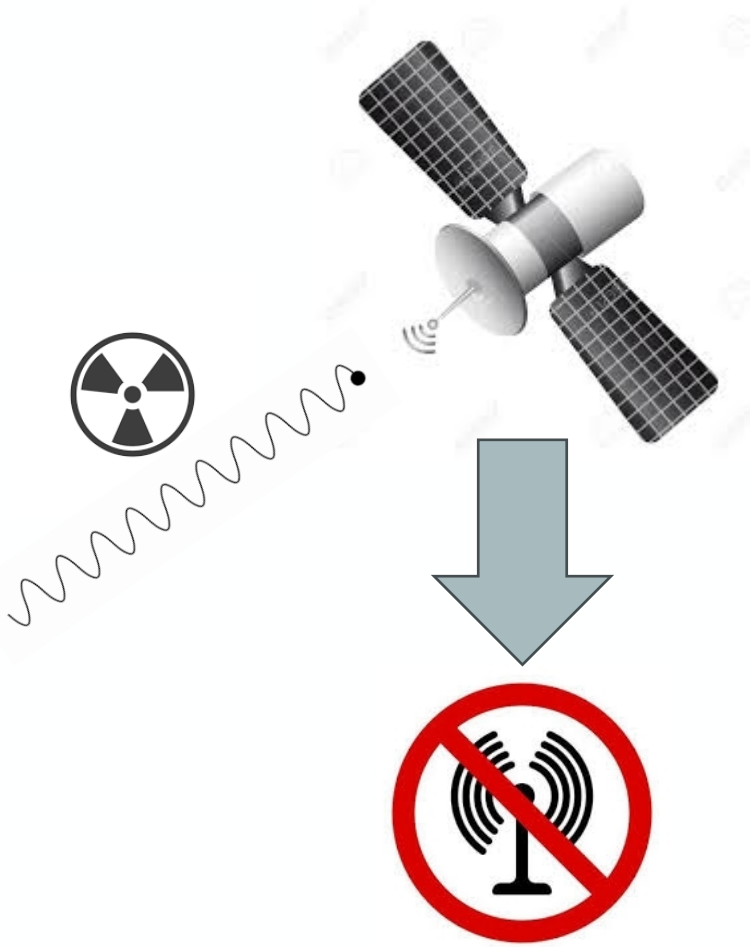
Introduction



Application: Semiconductors such as InSb, InGaAs, InAs, etc. are an attractive class of materials for infrared (IR) sensing due to their small bandgap

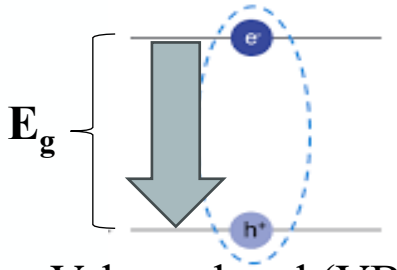
Working principle: Incident photons with energy proportional to the bandgap energy (E_g) will excite electrons to a higher energy state and generate an electrical current

Challenge: Radiation damage introduces defects that may alter IR device performance

Impact: New defect induced electronic states may result in IR device failure

Introduction

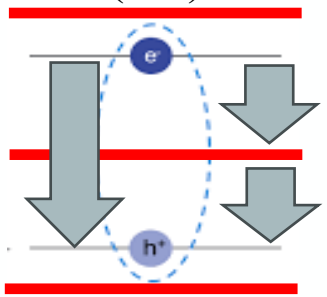
Conduction band(CB): electronic current



Valence band (VB)

Pristine
Defect free

Conduction band(CB): electronic current



Valence band (VB)

Defect induced NEW electronic relaxation pathways

- Defects introduce additional electronic states:
- Defects can change mechanical properties:
  - Electronic
  - Magnetic
  - Optical
- Defect electronic states may reside in:
  - the conduction band
  - the valence band
  - the bandgap
- Defect states in the bandgap :
  - Additional electronic relaxation pathway creates **recombination center** in the bandgap

Approach

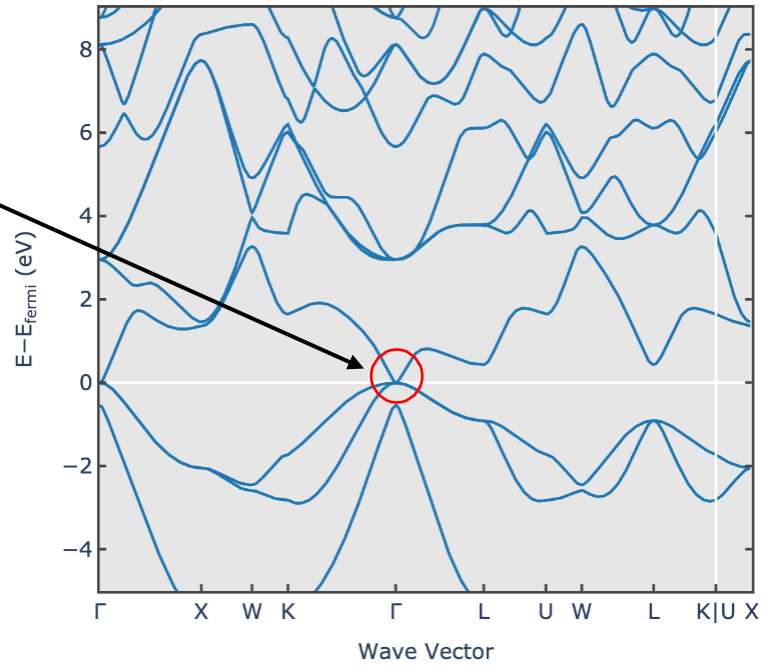
-**Observation**: Standard Density-Functional-Theory (DFT) erroneously predicts InSb to be metallic ($E_g = 0$ eV)

-**Experiment**: $E_g = 0.24$ eV at $T = 0$ K *(Littler and Seiger, 1985)*

-**Methodology**: Hubbard U+V extensions correct the over-delocalization of the electrons and consistently opens a narrow bandgap *(Lee and Son, 2020)*
U-parameter: Local Coulomb repulsion
V-parameter: Intersite Coulomb interaction

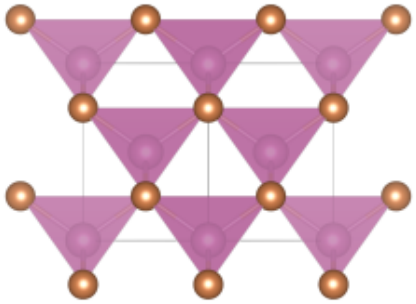
-**Significance**: An open bandgap allows us to study the electronic defect states introduced by radiation and determine where they reside

DFT InSb Materials Project



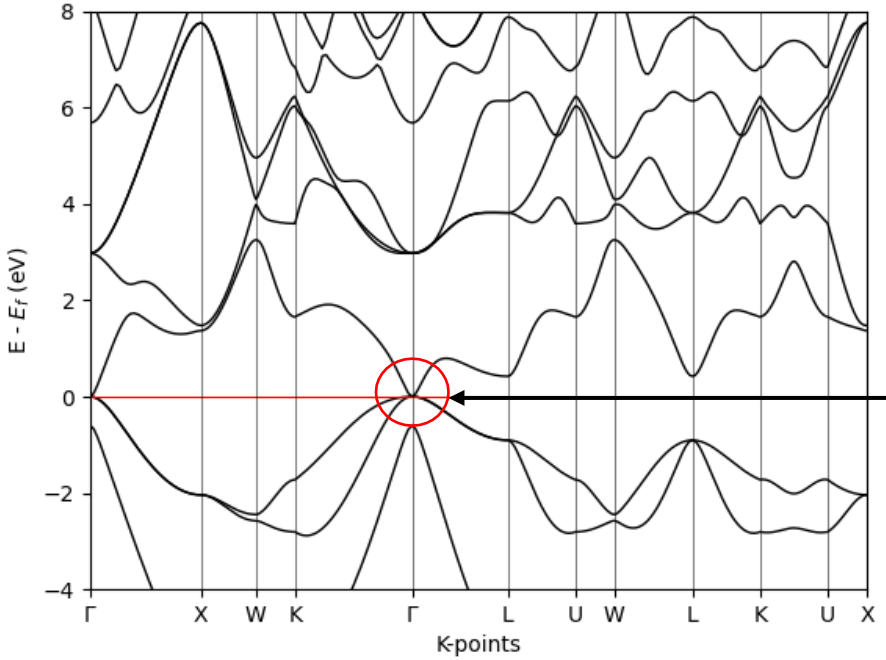
InSb (MP-20012)

Opening the Bandgap



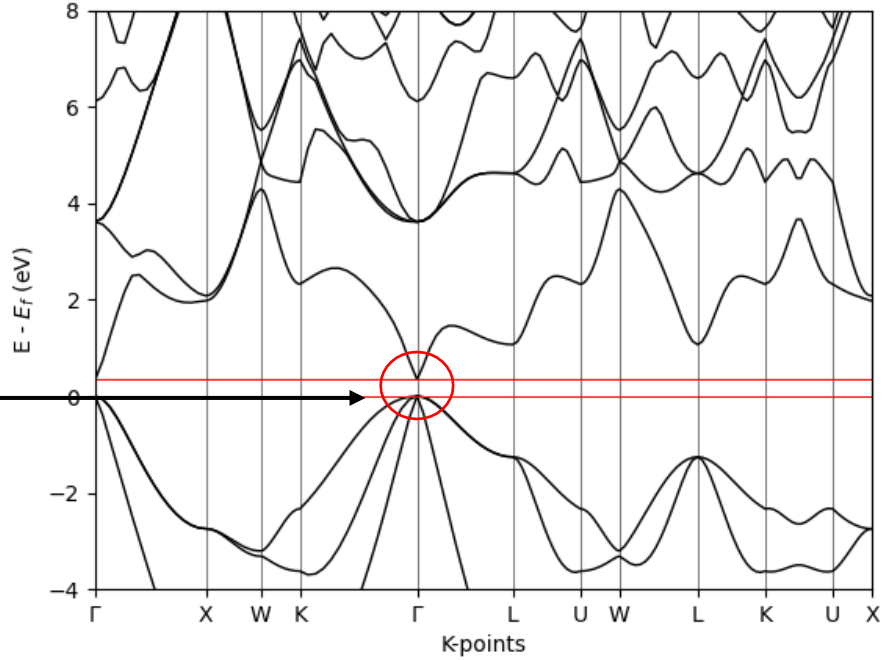
InSb

DFT InSb Primitive Cell



E_g = 0 eV **(Metallic)**

DFT+U+V InSb Primitive Cell



E_g = 0.36 eV

Expt. E_g = 0.24 eV at T = 0 K

(Littler and Seiger, 1985)

Insight:

- **DFT+U+V consistently opens the narrow bandgap of InSb**

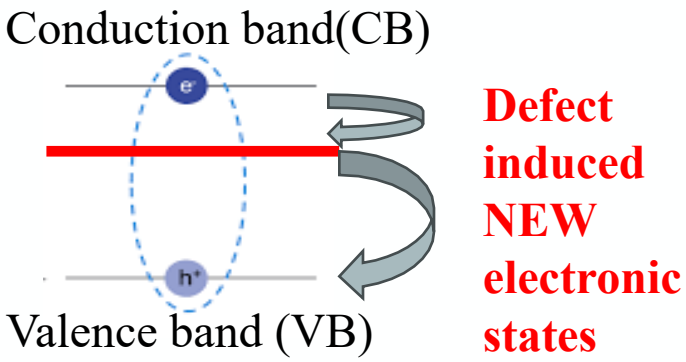
Point Defects 8-Atom InSb Antisite

Antisite: Substitutional defect

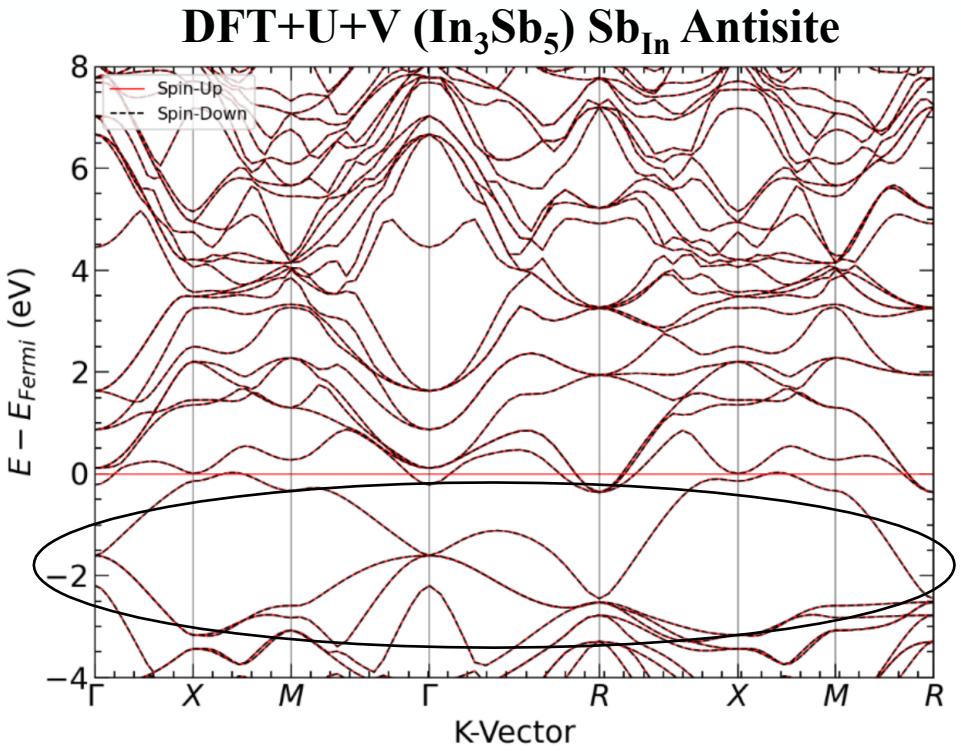
In → Sb (In_{Sb})

Sb → In (Sb_{In}) i.e., Electron Level 2 (EL2)

Vacancy: Atom is removed from the material



Defect induced NEW electronic states

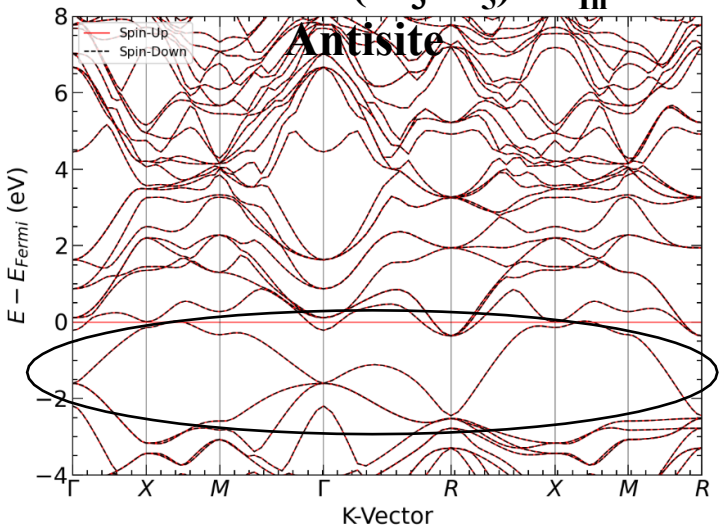


Insight:

- Large electronic dispersion
- Unclear if recombination center forms
- Need larger simulation cells

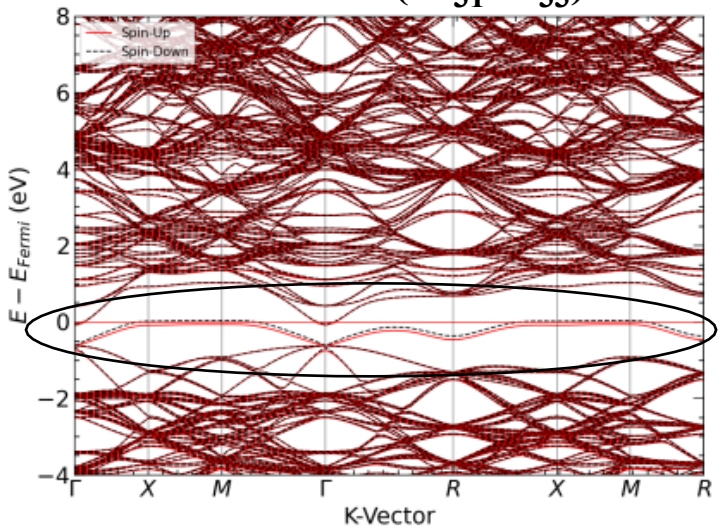
InSb 64-Atom Antisite Defects

DFT+U+V (In_3Sb_5) Sb_{In} Antisite



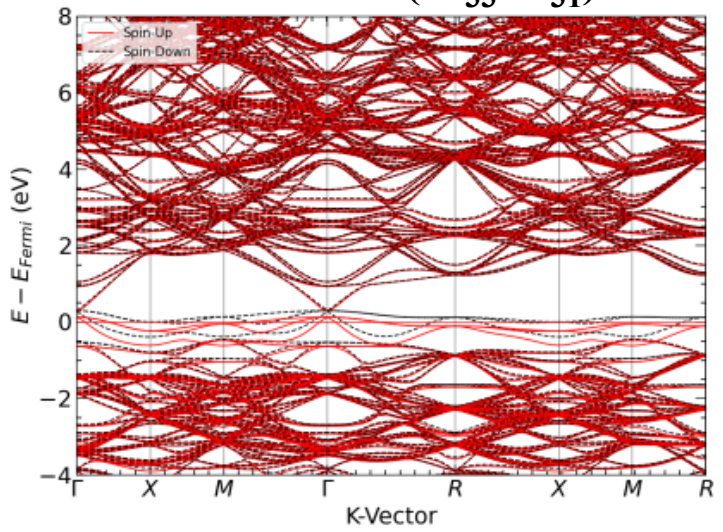
- Metallic
- **Large electronic dispersion**

DFT+U+V relaxed ($In_{31}Sb_{33}$) Antisite



- Metallic
- Added $2e^-$ → Fermi level shifted into CB
- **Less electronic dispersion**

DFT+U+V relaxed ($In_{33}Sb_{31}$) Antisite

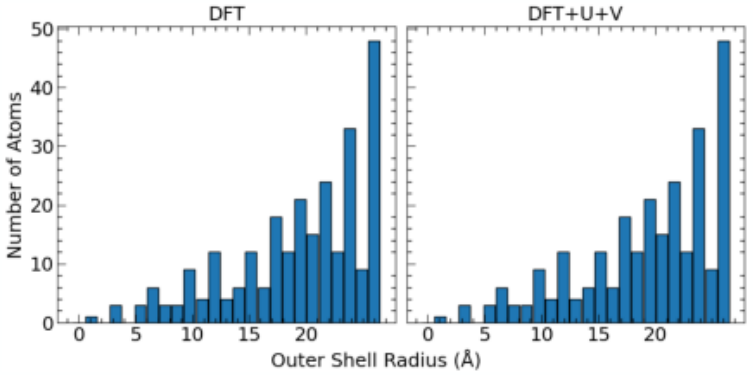


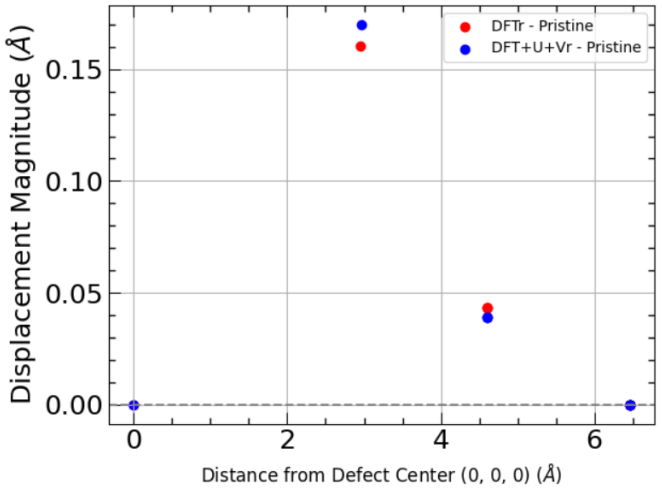
- Metallic
- Removed $2e^-$ → Fermi level shifted into VB
- Complicated defect states

Insight:

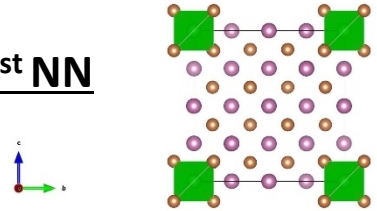
- **Dispersion has decreased in 64 atom simulations**
- **Dispersion still significant**

Analyzing 64-Atom Sb_{In} Ionic Displacements

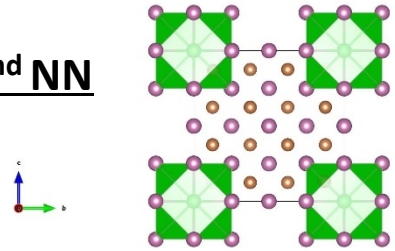




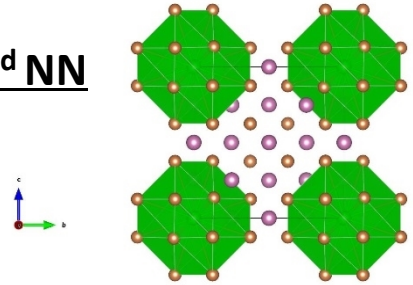
1st NN



2nd NN



3rd NN

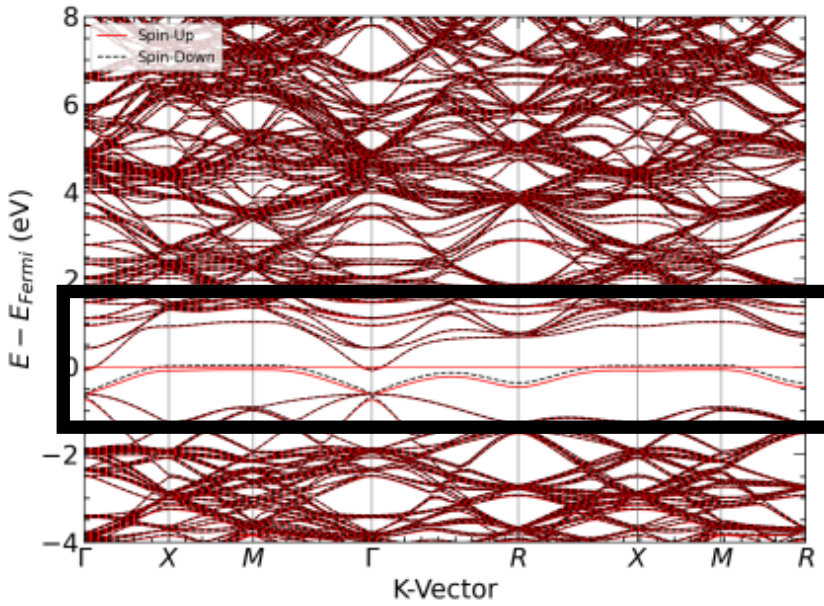


Insight:

- Displacement decreases with distance from the defect
- DFT and DFT+U+V exhibit similar defect relaxation patterns

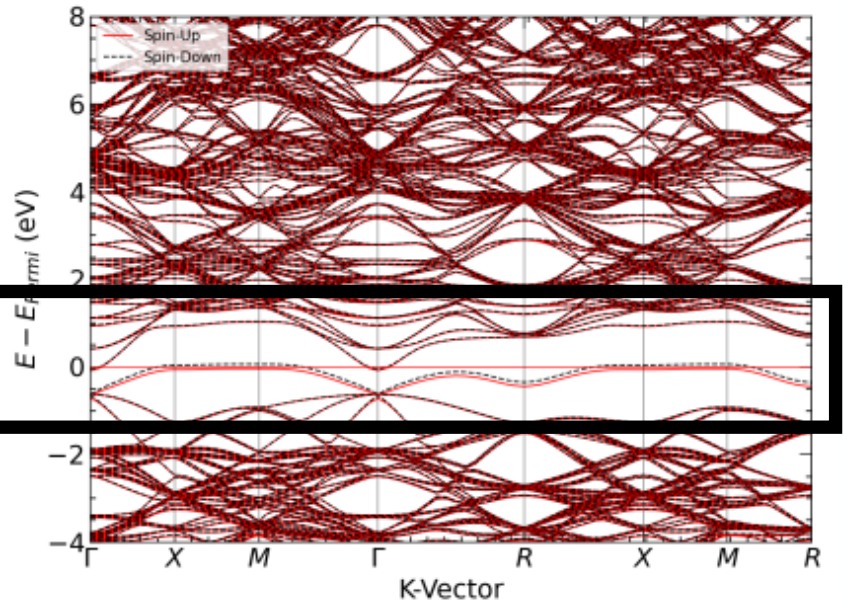
Analyzing DFT & DFT+U+V Relax Band Structures: 64-Atom Sb_{In} Antisite

DFT+U+V relax
DFT+U+V electronic structure



- VBM = -0.59 eV
- CBM = -0.09 eV
- E_g = 0.50 eV

DFT relax
DFT+U+V electronic structure



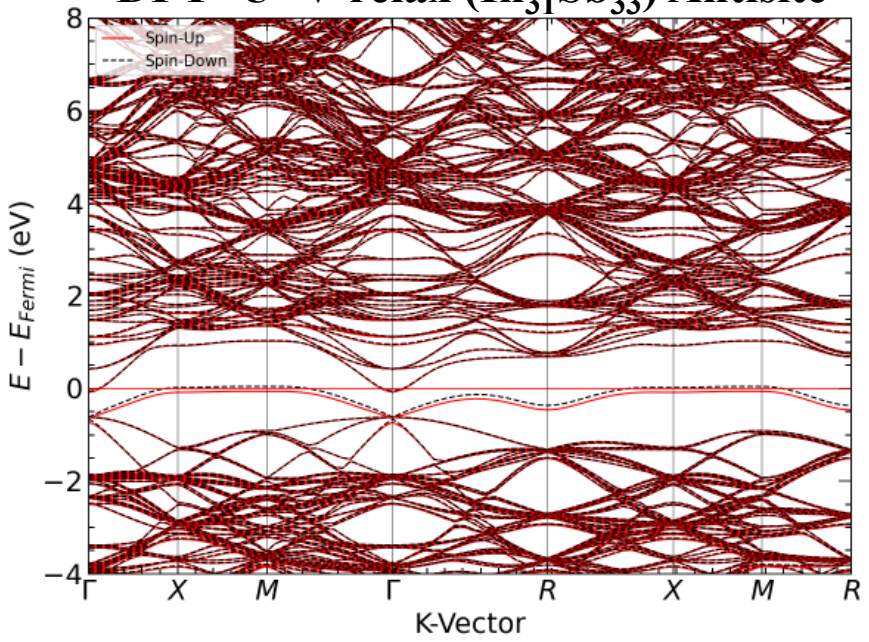
- VBM = -0.60 eV
- CBM = -0.09 eV
- E_g = 0.51 eV

Insight:

- **Electronic structure of DFT relax and DFT+U+V are nearly identical**
- **Combine DFT-relaxation (fast) and Hubbard U+V band structure (slow) calculation**

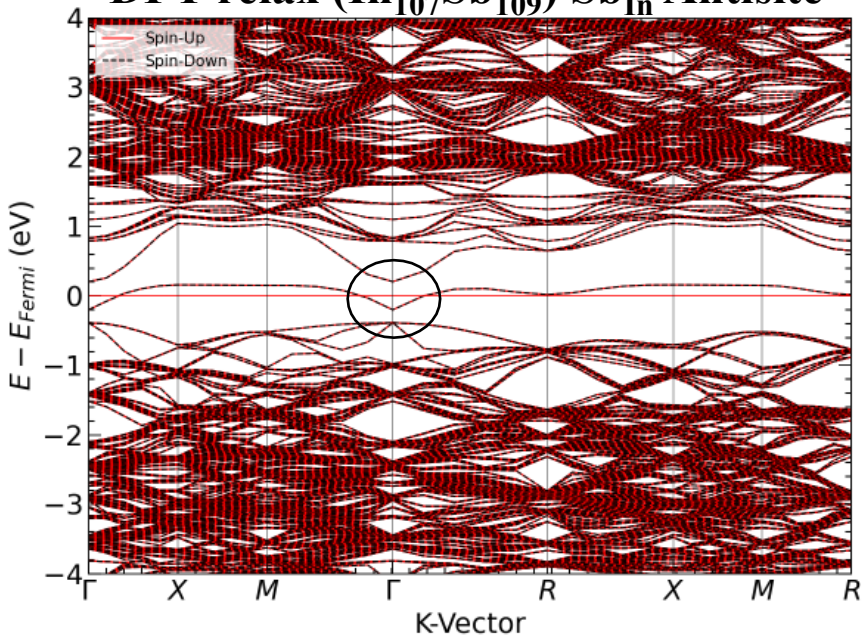
216-Atom Sb_{In} Antisite Defect

DFT+U+V-relax ($In_{31}Sb_{33}$) Antisite



64-Atoms

DFT-relax ($In_{107}Sb_{109}$) Sb_{In} Antisite



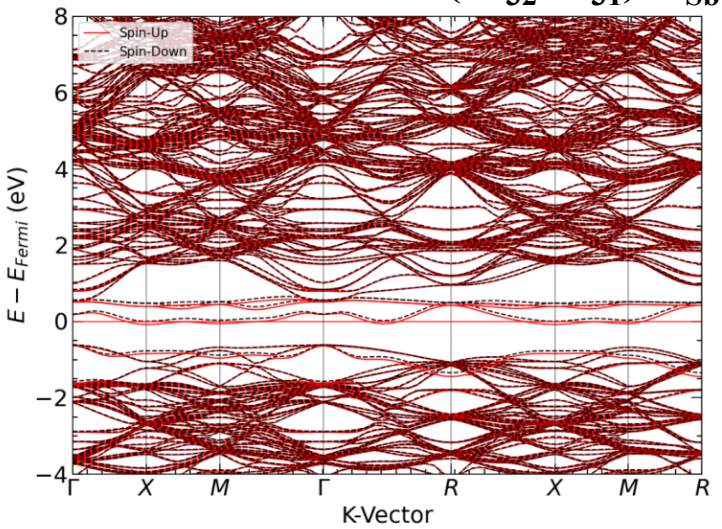
216-Atoms

Insight:

- Electronic dispersion decreases
- Defect electronic state is entirely in the bandgap
- Formation of recombination center
- Additional electronic relaxation pathway

InSb 64-Atom Vacancy Defects

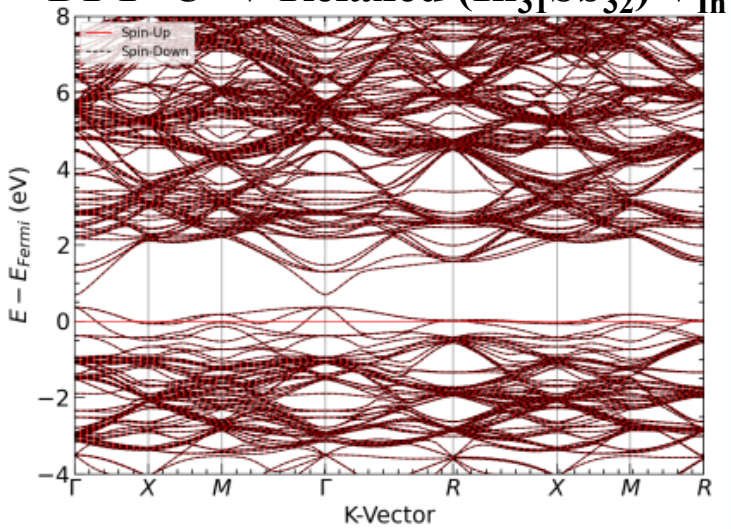
DFT+U+V Relaxed ($In_{32}Sb_{31}$) V_{Sb}



- Metallic
- Removed $5e^-$ → Fermi level shifted into bandgap

Electronic states in the bandgap → recombination center

DFT+U+V Relaxed ($In_{31}Sb_{32}$) V_{In}



- Metallic
- Removed $3e^-$ → Fermi level shifted into VB

Electronic states not in the bandgap → no recombination center

Insight:

V_{Sb}: Defect state in bandgap, forms recombination center

V_{In}: Defect state not in bandgap, does not form recombination center

Formation of recombination center depends on geometry and chemical nature of defect

Summary

- Defect bands can create recombination centers in the bandgap of the host material:
  - Small simulation cells show significant electronic dispersion from defect-defect interactions
  → Cannot conclude with certainty if recombination center forms

  - Larger simulation cells decrease electronic dispersion
    - Antisite Sb_{In}: **will form recombination center**
    - Vacancy V_{Sb}: **will form recombination center**
    - Vacancy V_{In}: **no recombination center**
    - Antisite In_{sb}: complicated electronic structure, recombination center?

Successfully computed electronic structure of point defects in small gap materials, needed for the evaluation of electronic devices and infrared detector reliability in radiation environments

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