Abinit Project

SGTB Khalsa College, University of Delhi

Preetpal Singh(2020PHY1140)(20068567043)

Unique Paper Code: 32221502

Paper Title: Solid State Physics

Submitted on: October 20, 2022

B.Sc(H) Physics Sem V

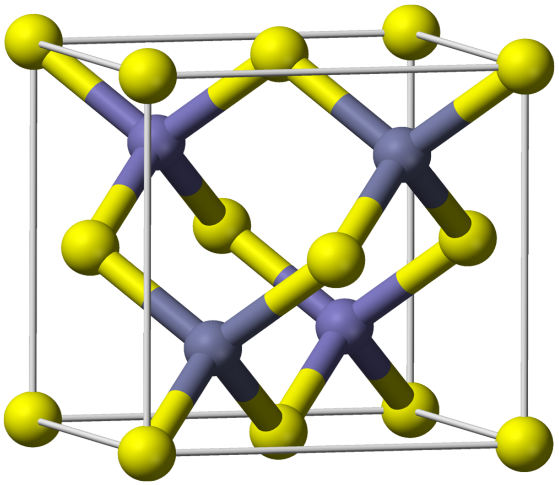
Submitted to: Dr. Kuldeep Kumar

1 Aim

To study variation in band gap of InAs by changing lattice parameter c with the using of Abinit.

2 Theory

Indium arsenide(InAs) is a narrow-bandgap semiconductor which is composed of indium and arsenic. It has FCC structure and band gap of 0.35 at room temperature.



Primitive vectors for fcc Structure

$$\overrightarrow{a_1} = \frac{a}{2}(\widehat{x} + \widehat{y}); \overrightarrow{a_2} = \frac{a}{2}(\widehat{y} + \widehat{z}); \overrightarrow{a_3} = \frac{a}{2}(\widehat{x} + \widehat{z})$$

The Resiprocal vectors for fcc Structure

$$\overrightarrow{b_1} = \frac{2\pi}{a}(-\widehat{x} + \widehat{y} + \widehat{z}); \overrightarrow{b_2} = \frac{2\pi}{a}(\widehat{x} - \widehat{y} + \widehat{z}); \overrightarrow{b_3} = \frac{2\pi}{a}(\widehat{x} + \widehat{y} - \widehat{z})$$

Brillouin zone

Critical points	FCC Structure
K	Middle of an edge joining two hexagonal faces
L	Center of a hexagonal face
U	Middle of an edge joining a hexagonal and a square face
W	Corner point
X	Center of a square face

Path: L-Γ-X-W-K

kptbounds for FCC

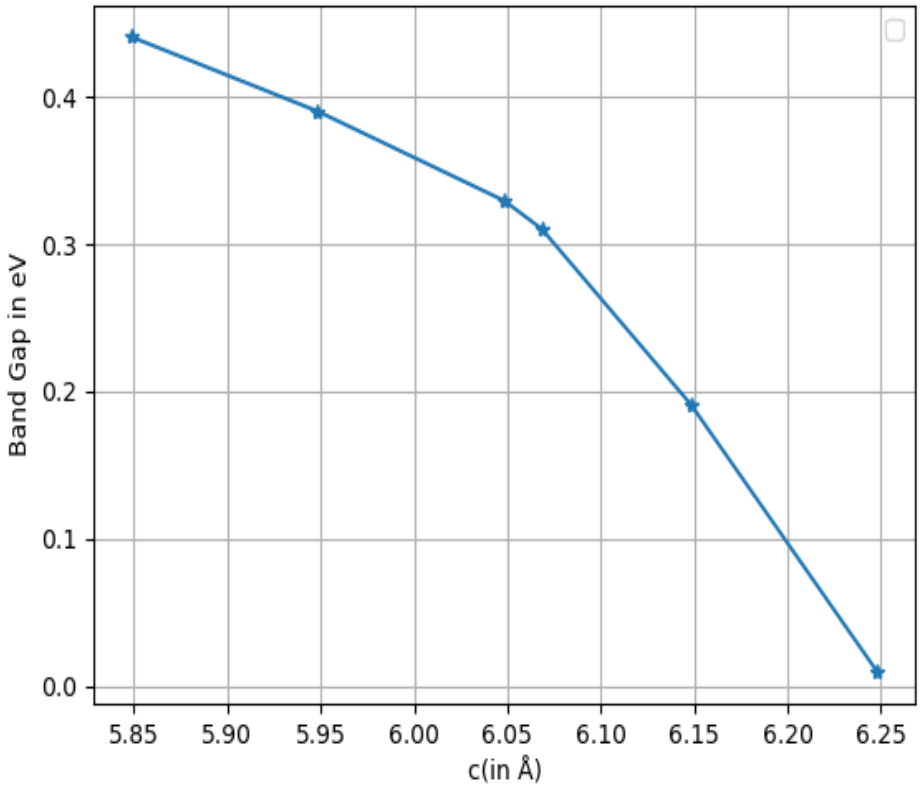
Critical Points	kptbounds
L	1/2 0 0
Γ	0 0 0
X	0 1/2 1/2
W	1/4 1/2 3/4
K	3/8 3/8 3/4

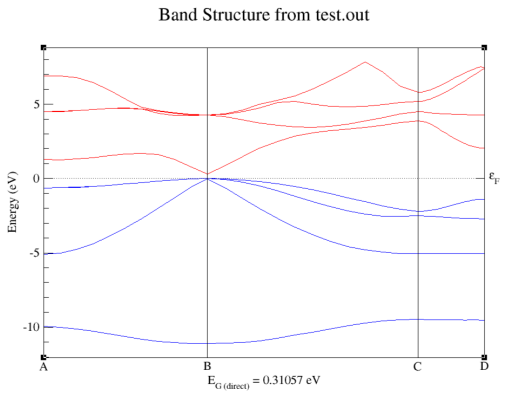
Variation of Band Gap with lattice parameter(c)

c(in Å)	Bandgap(in eV)
5.8483	0.44096
5.9483	0.39037
6.0483	0.32961
6.0583	0.329609
6.0683	0.31057
6.1483	0.19122
6.2483	0.00938

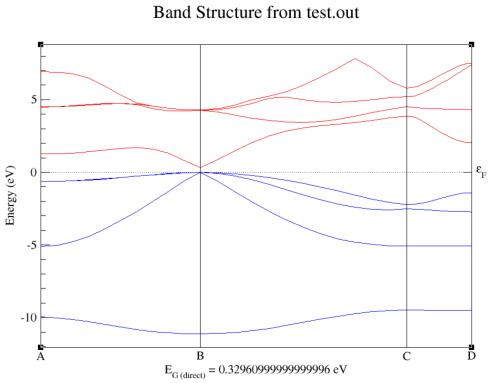
Table 1: Variation of Band Gap with c

Here, From the above table we can see that as the value of c is increased, Band Gap reduces because the interatomic distance is increased accordingly. Therefore, Force between parent atom and valence band decreases.

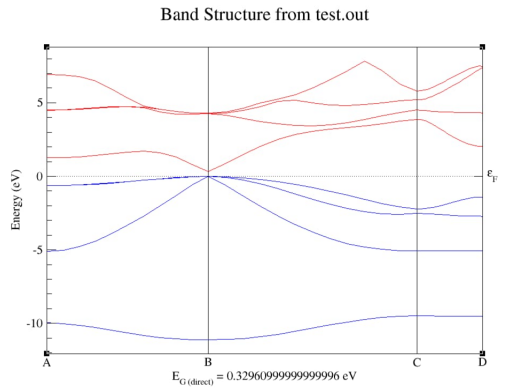




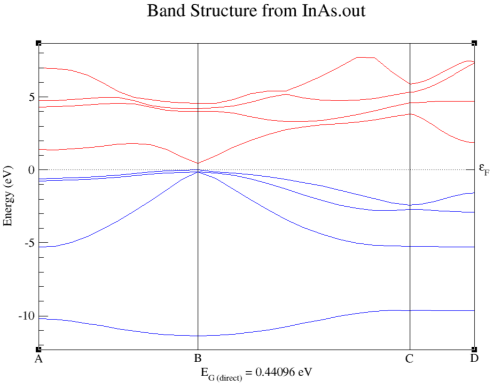
(a) c=6.0683



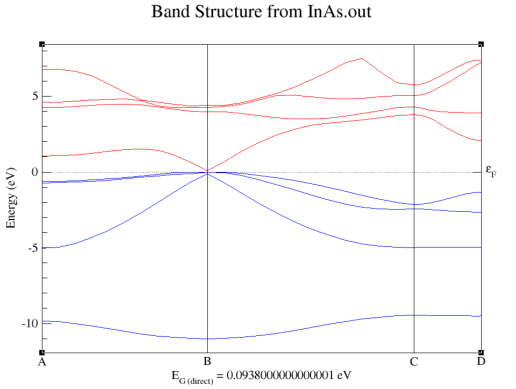
(b) c=6.0583



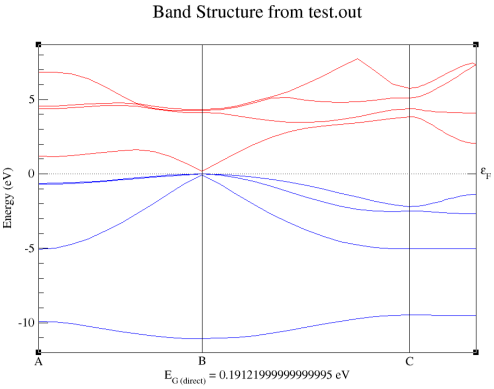
(a) c=6.0483



(b) c=5.8483



(a) c=6.2483



(b) c=6.1483