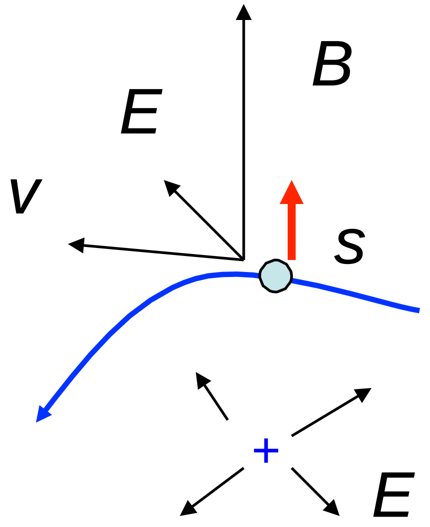
Origin of the spin-orbit interaction



Mott 1927

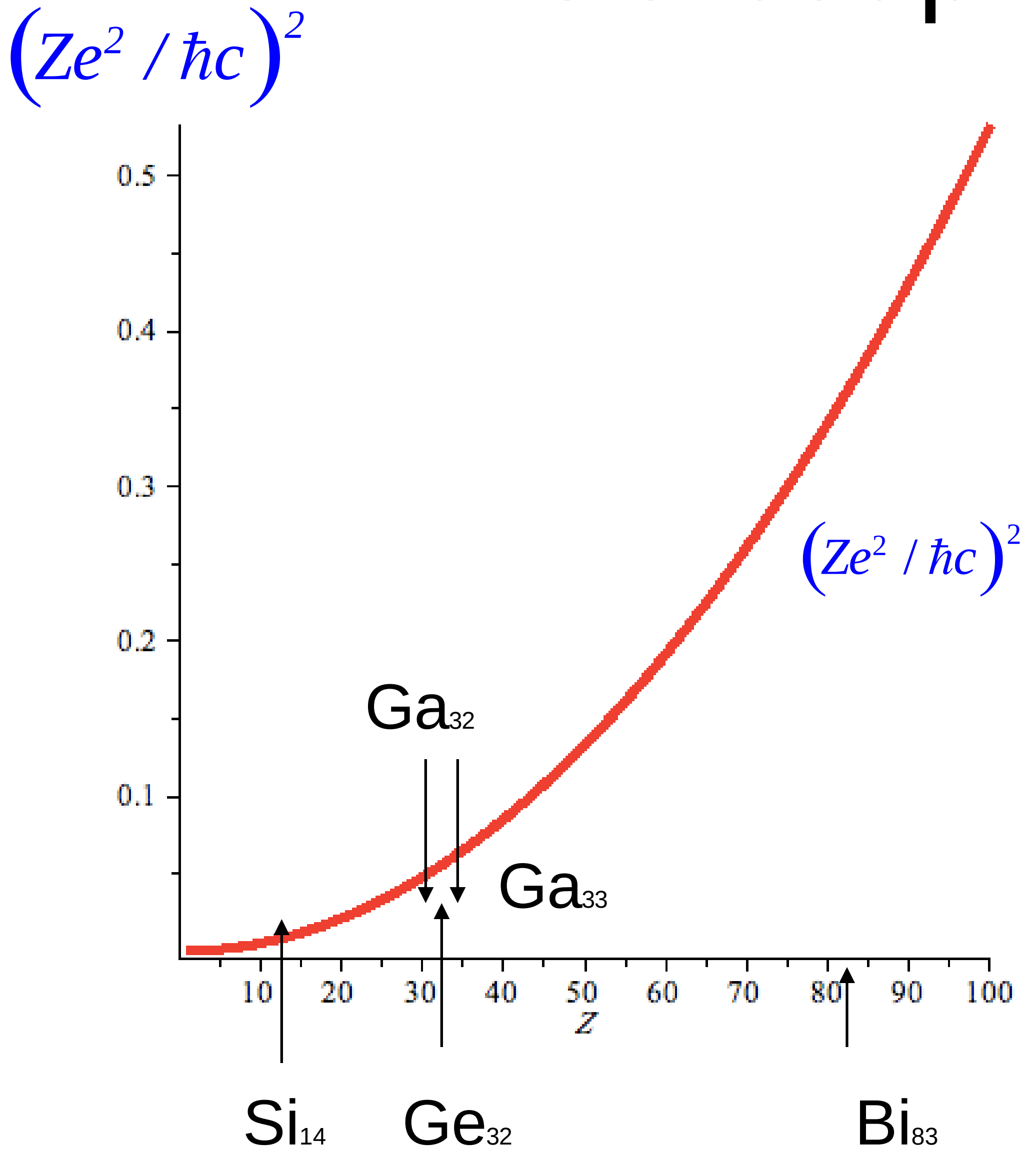
In a frame associated with the electron: $\mathbf{B} = \frac{1}{c}\mathbf{E}\times\mathbf{v} = \frac{1}{mc}\mathbf{E}\times\mathbf{p}$

Zeeman energy in the SO field: $\hat{H} = \frac{\mu_B}{mc}\vec{\sigma}\bullet(\mathbf{E}\times\hat{\mathbf{p}}) = -\frac{i\hbar^2}{2m^2c^2}\vec{\sigma}\bullet(\vec{\nabla}V\times\nabla)$

1/c expansion of the Dirac equation

$$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m} + eV}_{\text{non-relativistic}} + \underbrace{\frac{\hat{p}^4}{8m^2c^2}}_{\text{K.E. correction}} + \underbrace{\frac{\hbar^2}{8m^2c^2}\nabla^2 V}_{\text{Darwin term}} + \underbrace{\frac{\hbar}{4m^2c^2}\vec{\sigma}\bullet(\vec{\nabla}V \times \hat{\mathbf{p}})}_{\text{SOI}}$$

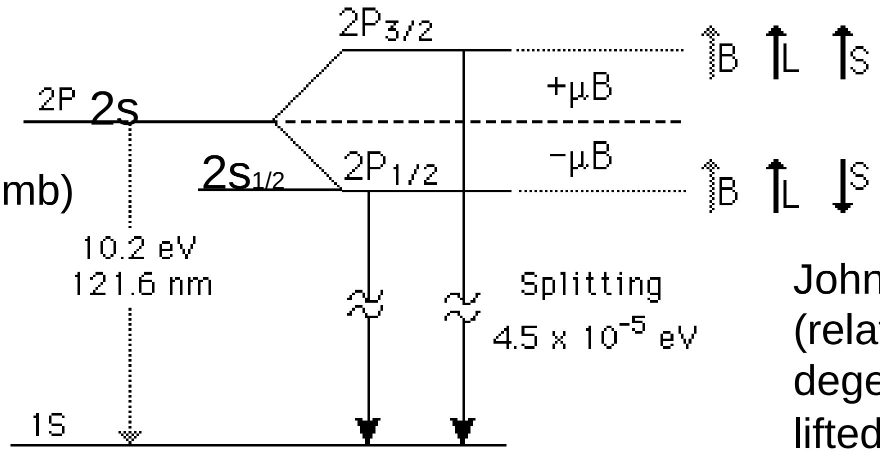
SO coupling



$(Ze^2/\hbar c)^2$	Si_{14}	Ga_{31}	Ge_{32}	As_{33}	Bi_{83}
	0.01	0.051	0.055	0.058	0.38

Fine structure of atomic levels

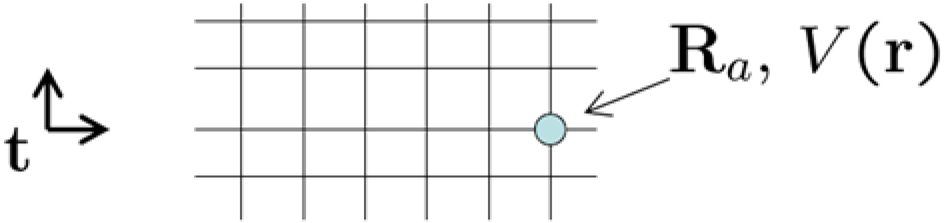
Hydrogen



Runge-Lentz
(non-relativistic Coulomb)
+spin degeneracy

Johnson-Lippman
(relativistic Coulomb)
degeneracy
lifted by radiation corrections
(Lamb shift)

Spin-orbit coupling



$$V_{so}(\mathbf{r}) = \frac{\hbar}{4m^2c^2}\nabla V_{sc} \times \mathbf{p}\cdot\sigma, \qquad V_{sc}(\mathbf{r}) = \sum_a V\left(\mathbf{r}-\mathbf{R}_a\right)$$

for spherically symmetric ionic potentials,

$$V_{so}(\mathbf{r}) = \lambda(\mathbf{r})\,\hat{\mathbf{l}}\cdot\sigma, \qquad \lambda(\mathbf{r}+\mathbf{t}) = \lambda(\mathbf{r})$$

periodic!!!

Time reversal symmetry

$$\begin{array}{ccc} t & \longrightarrow & -t \\ l & \longrightarrow & -l \\ \sigma & \longrightarrow & -\sigma \end{array}$$

⬇

$$V_{so} \sim l\cdot\sigma \longrightarrow V_{so}$$

SOC preserves time reversal symmetry!

- Kramers (spin) degeneracy

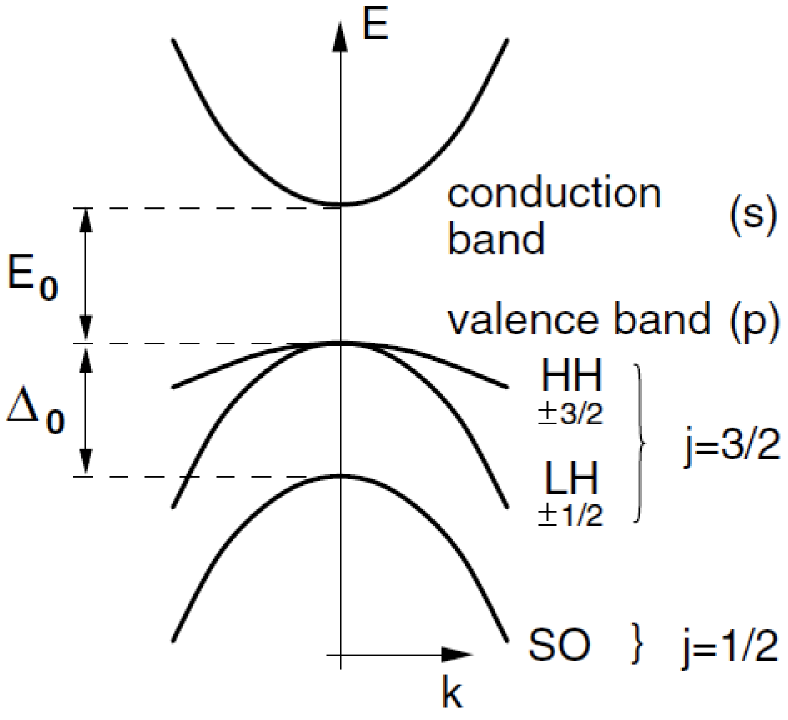
Two types of SOI in solids

1) <u>Symmetry-independent:</u>
   exists in all types of crystals
   stem from SOI in atomic orbitals

2) <u>Symmetry-dependent:</u>
   exists only in crystals without inversion symmetry
   a) Dresselhaus interaction (bulk): Bulk-Induced-Assymetry (BIA)
   b) Bychkov-Rashba (surface): Surface-Induced-Asymmetry (SIA)

Example of symmetry-independent SOI: SO-split-off valence bands

Winkler, Ch. 3



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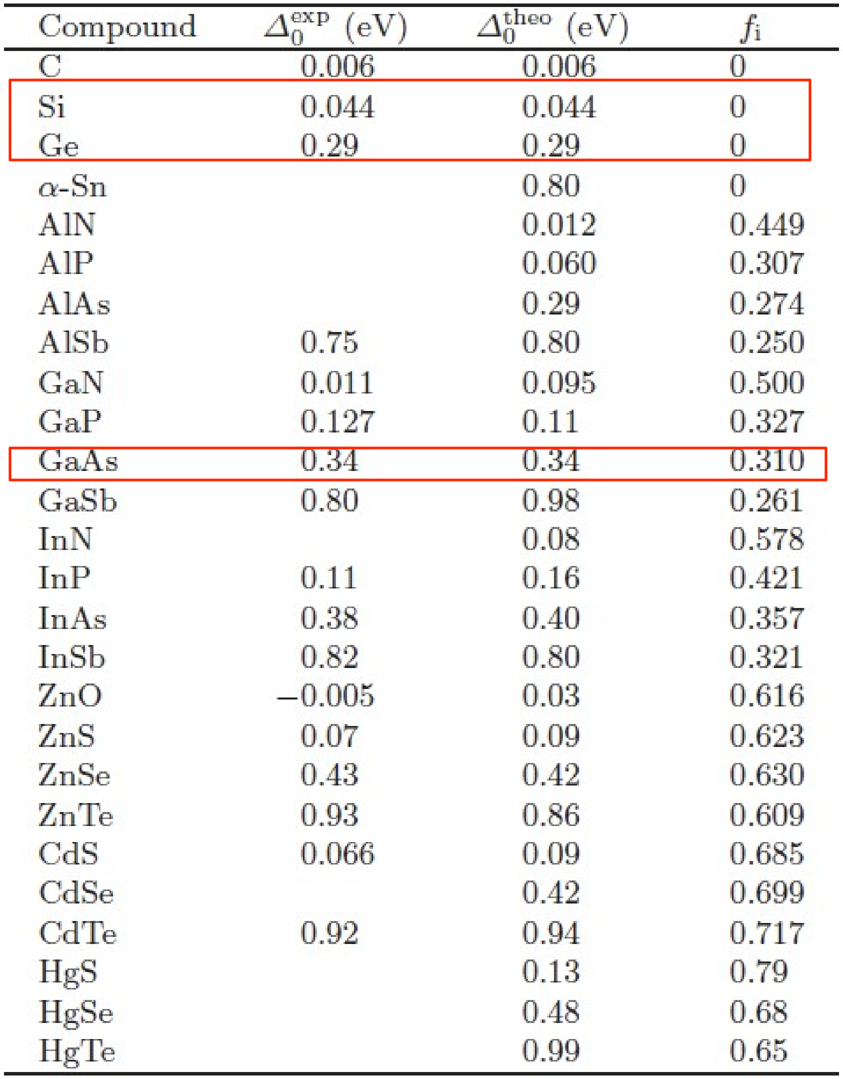
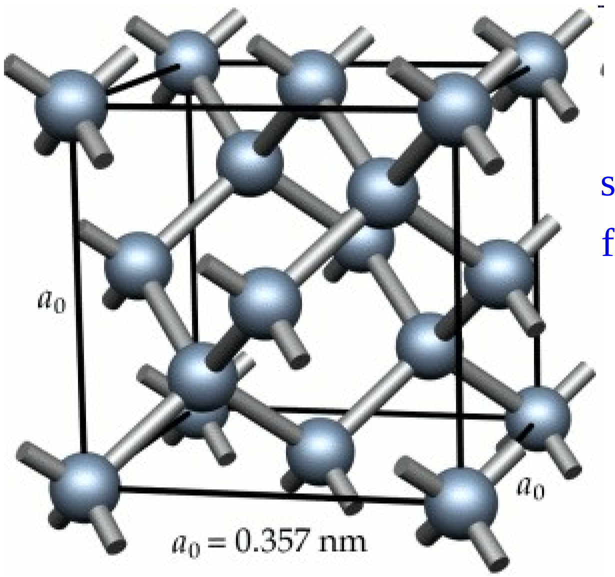


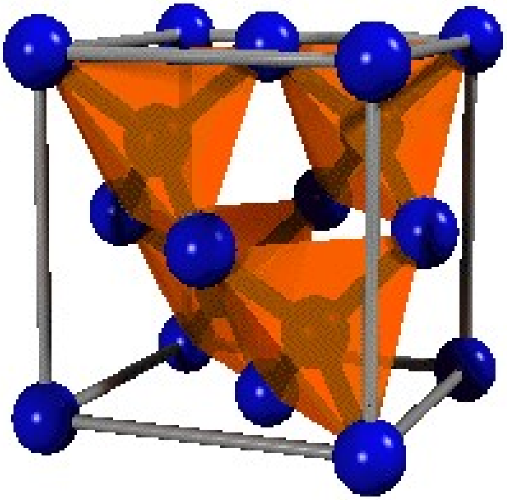
Compound	Δ_0^{exp} (eV)	Δ_0^{theo} (eV)	f_i
C	0.006	0.006	0
Si	0.044	0.044	0
Ge	0.29	0.29	0
α-Sn		0.80	0
AlN		0.012	0.449
AlP		0.060	0.307
AlAs		0.29	0.274
AlSb	0.75	0.80	0.250
GaN	0.011	0.095	0.500
GaP	0.127	0.11	0.327
GaAs	0.34	0.34	0.310
GaSb	0.80	0.98	0.261
InN		0.08	0.578
InP	0.11	0.16	0.421
InAs	0.38	0.40	0.357
InSb	0.82	0.80	0.321
ZnO	−0.005	0.03	0.616
ZnS	0.07	0.09	0.623
ZnSe	0.43	0.42	0.630
ZnTe	0.93	0.86	0.609
CdS	0.066	0.09	0.685
CdSe		0.42	0.699
CdTe	0.92	0.94	0.717
HgS		0.13	0.79
HgSe		0.48	0.68
HgTe		0.99	0.65

Non-centrosymmetric crystals

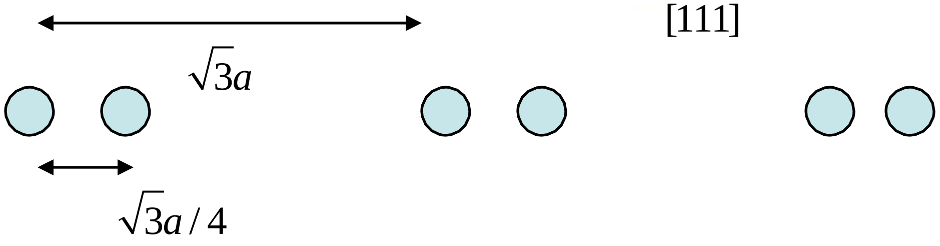


space group: O_h^7 (non-symmorphic)

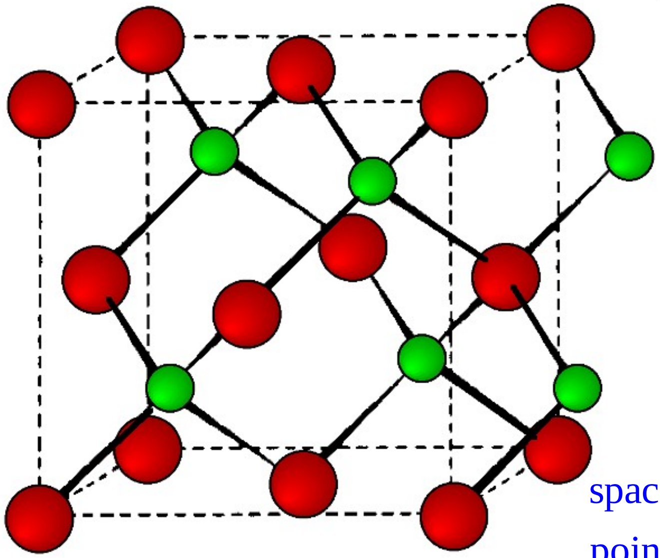
factor group $O_h = T_d \times I$

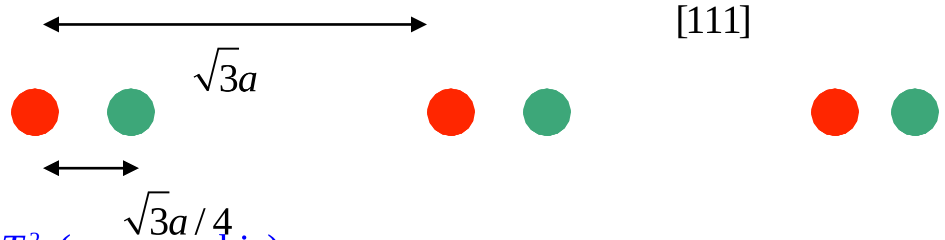


S. Sque (Exter)



Diamond (C): Si, Ge





space group: T_d^2 (symmorphic)

point group: T_d (methane CH_4)

Zincblende (ZnS): GaAs, GaP, InAs, InSb, ZnSe, CdTe …

Additional band splitting in non-centrosymmetric crystals

Kramers theorem: if time-reversal symmetry is not broken, all eigenstates are at least doubly degenerate

if ψ is a solution, ψ^* is also solution

Kramers doublets $\varepsilon_s(\mathbf{k})$, $s = \pm 1$ (not necessary spin projection!)

Time reversal symmetry: **k→-k,** t → -t $\varepsilon_s(\mathbf{k}) = \varepsilon_{-s}(-\mathbf{k})$

No SOI: $\varepsilon(\mathbf{k}) = \varepsilon(-\mathbf{k})$ regardless of the inversion symmetry

With SOI: i) If a crystal is centrosymmetric

$$\varepsilon_s(\mathbf{k}) \underbrace{=}_{t\to -t} \varepsilon_{-s}(-\mathbf{k}) \underbrace{=}_{\mathbf{k}\to -\mathbf{k}} \varepsilon_{-s}(\mathbf{k}) \Rightarrow \varepsilon_s(\mathbf{k}) = \varepsilon_{-s}(\mathbf{k})$$

ii) If a crystal is non-centrosymmetric,

$\varepsilon_s(\mathbf{k}) \neq \varepsilon_{-s}(\mathbf{k})$ B=0 “spin” splitting