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All electron Band structure CAlculation Package

— ABCAP —

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LDA and LDA+U method

Full potential

Linearized APW basis

Space-group analysis by TSPACE

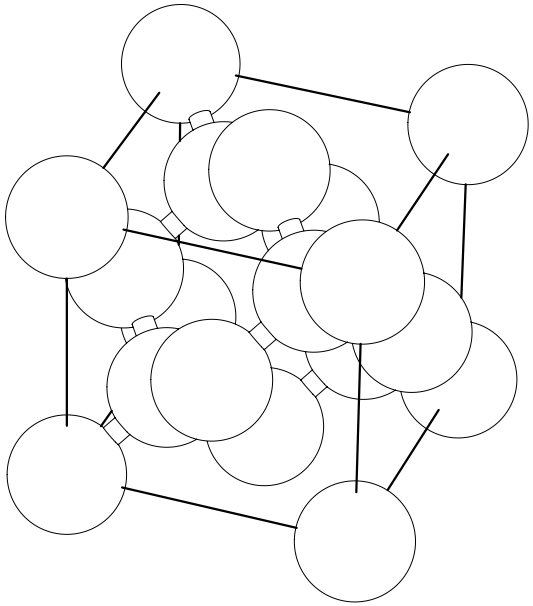
Optical-constant and Thermoelectric-power calculation

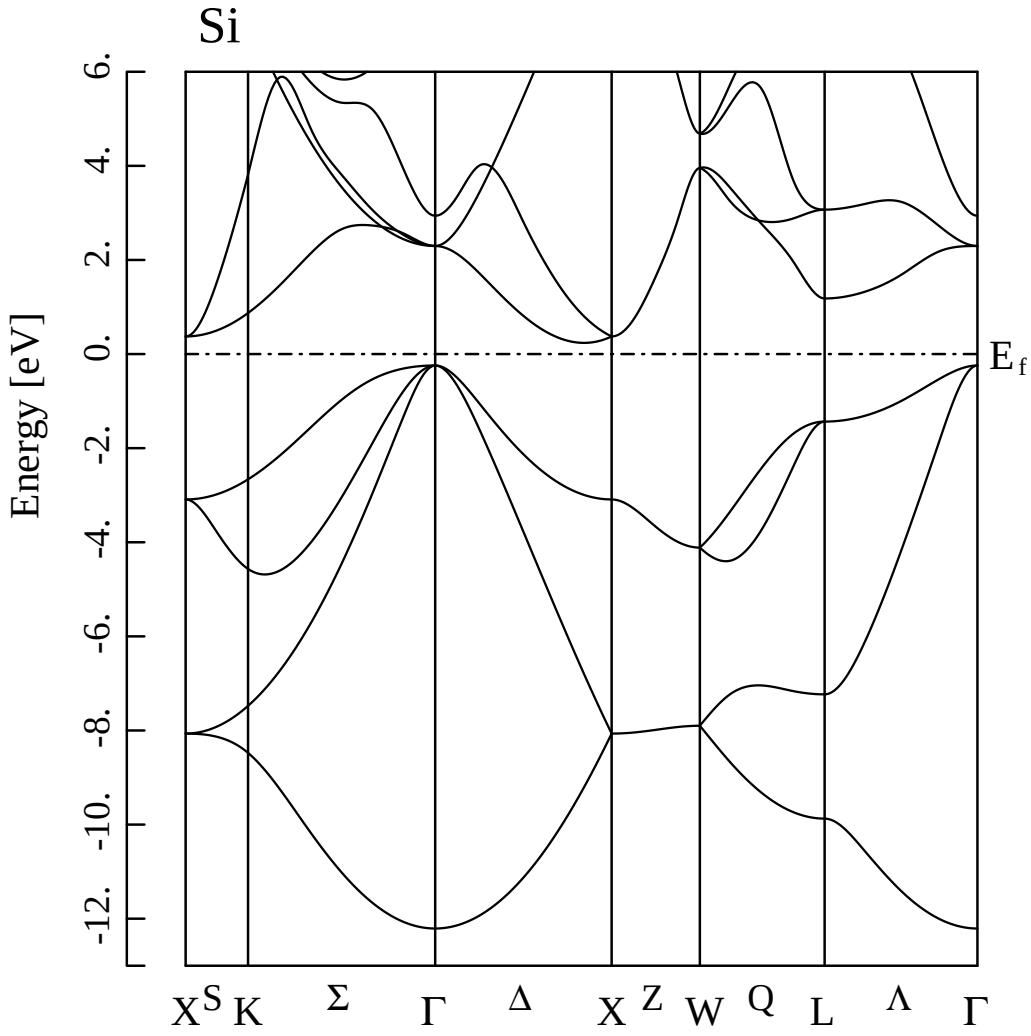
Silicon (Si)

Band structure : $\epsilon(\boldsymbol{k})$

$\hbar\boldsymbol{k}$: crystal momentum ($\boldsymbol{k}$: crystal wave number)

Crystal structure

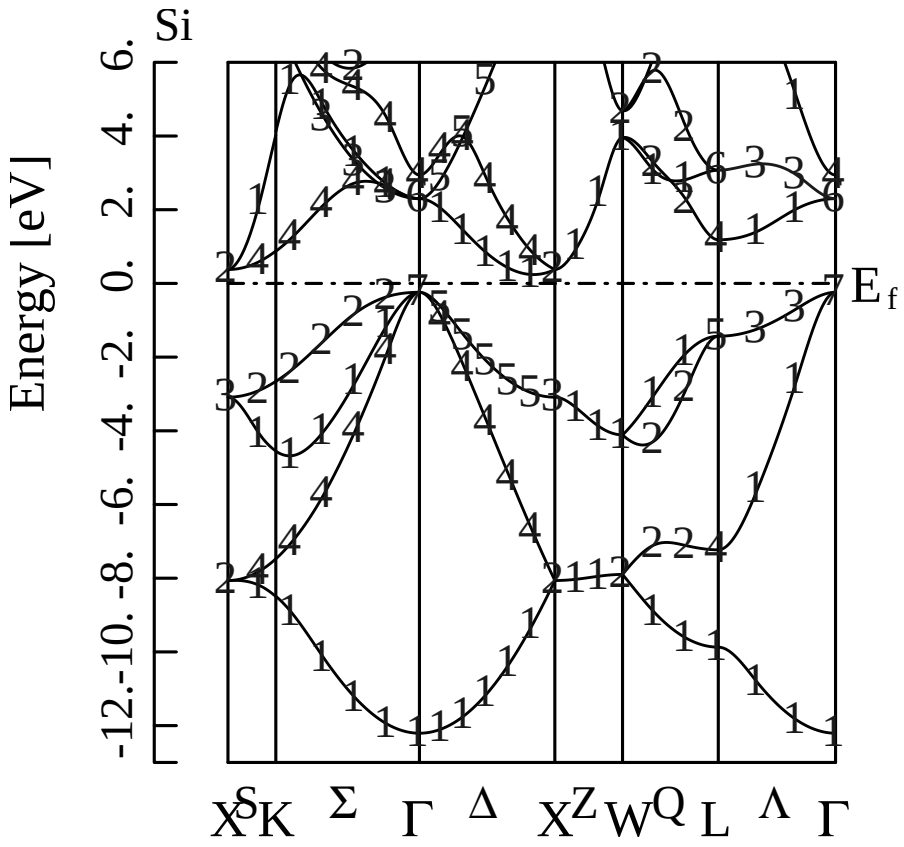




```
Input for Si (diamond)  ---ab_prp.data---
lattice parameter -2----*----3----*----4----*----5----*----6----*---
5.4296 5.4296 5.4296  90.0 90.0 90.0 !a,b,c[A], alpha,beta,gamma
space group       -2----*----3----*----4----*----5----*----6----*---
 3   2   3   0                !idim, il(R,H,P(1),F,I,C,A,B),ngen,inv
    5   0 1  0 1  0 1                              !igen,jgen(2,3)
   19   1 4  1 4  1 4                              !igen,jgen(2,3)
   25   1 4  1 4  1 4                              !igen,jgen(2,3)
kinds of atoms    -2----*----3----*----4----*----5----*----6----*---
 1                                                 !# of kinds
 1   0.0        0.0        0.0       Si           !jpos,position,name
magnetic state    -2----*----3----*----4----*----5----*----6----*---
 0                                                 !jmag(0,1,2)
k-points (# of division)  ---3----*----4----*----5----*----6----*---
  8  8  8                             !nx,ny,nz
!---*----1----*----2----*----3----*----4----*----5----*----6----*---
```

```
Atomic data ---atom.data---
-----------------------------------
H
 1.0   1    1.0079  1.0
105
0.5
0.5
-----------------------------------
Si
14.0   5   28.086   2.0
100 200 210 305 315
1.0 1.0 3.0 1.0 1.0
1.0 1.0 3.0 1.0 1.0
-----------------------------------
```

Symmetry of eigenenergy states

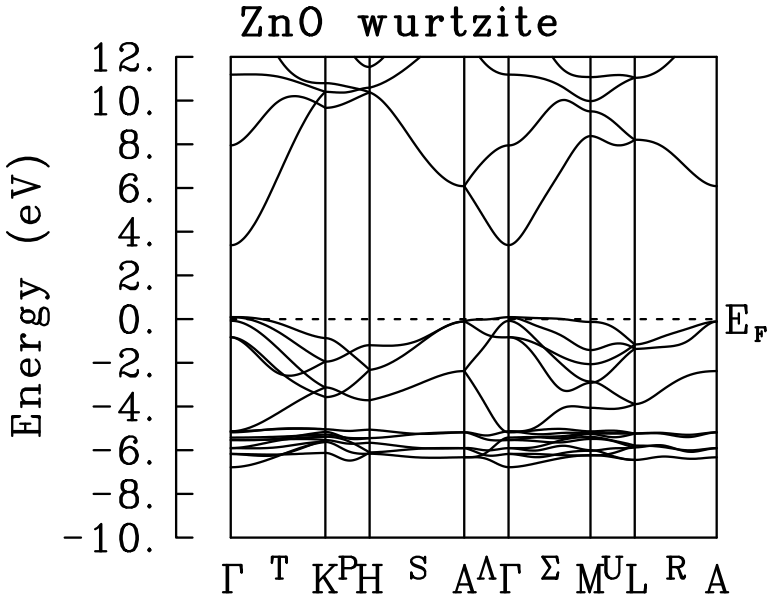


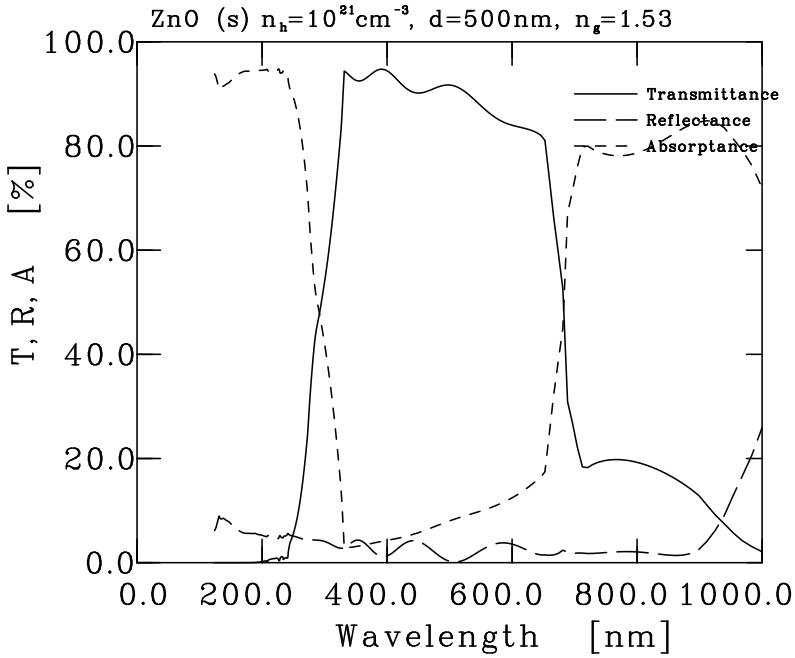
Irreducible representations at the Γ point

TSPACE	BSW		basis f.
1	Γ_1	Γ_1	1
4	Γ'_2	Γ_2^-	xyz
6	Γ_{15}	Γ_{15}^-	x, y, z
7	Γ'_{25}	Γ_{25}^+	xy, yz, zx
9	Γ_{12}	Γ_{12}^+	$x^2 - y^2, z^2$

BSW:

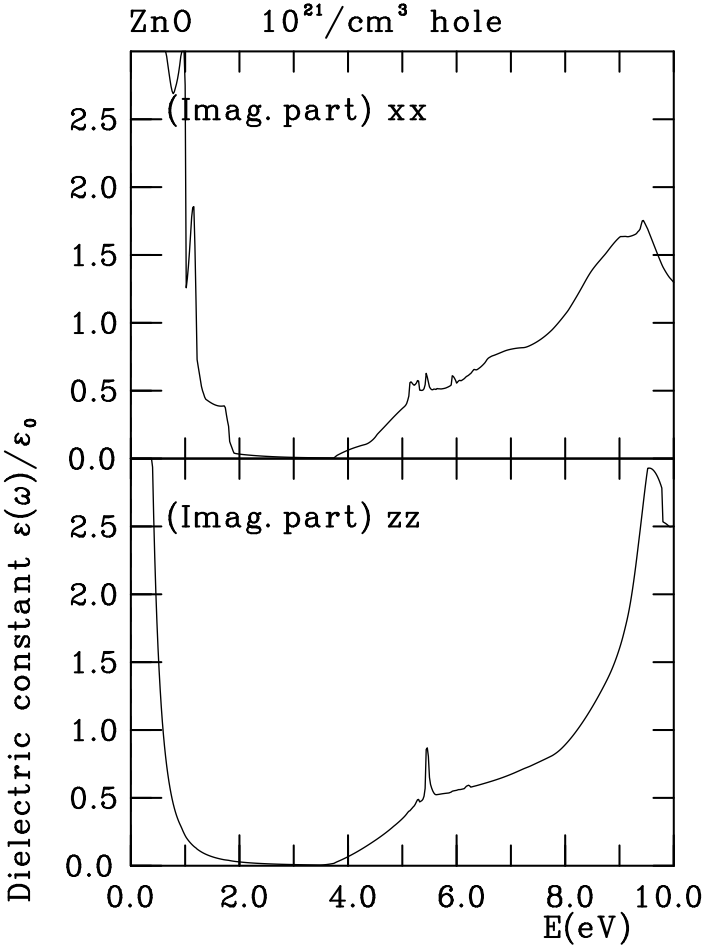
L. P. Bouckaert, R. Smoluchowski, and E. Wigner, Phys. Rev. 50 , 58 (1936).





hole-doped ZnO

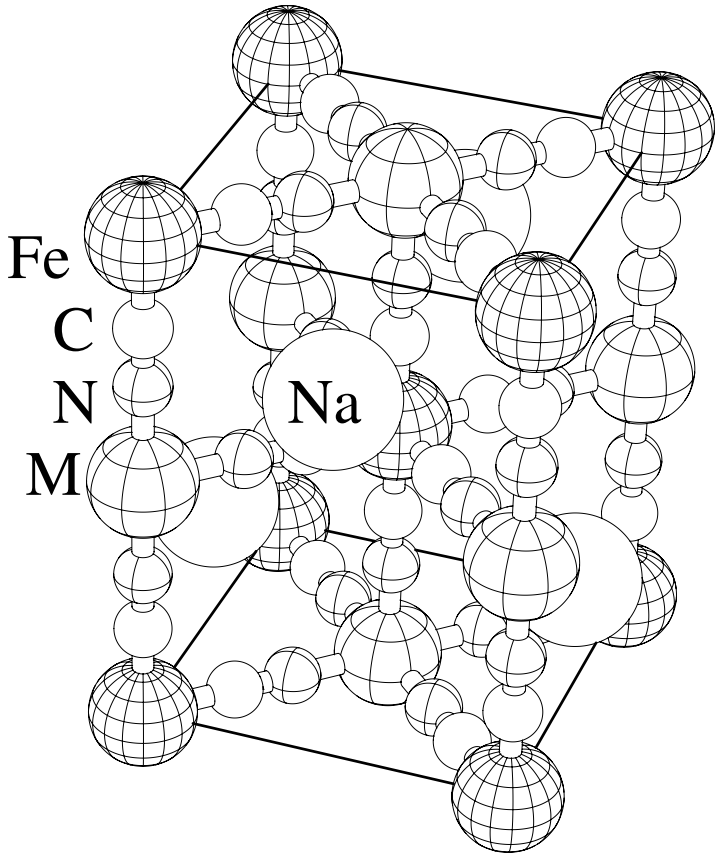
Im $\varepsilon(\omega)$



Visible light : 1.7eV ~ 3.1eV

730nm ~ 400nm

Crystal Structure of NaMFe(CN)$_6$ (M =Fe, Co, Ni)



Assumed structure

- bct (fcc: a =9.8Å, 10.0Å)
- Interatomic distances

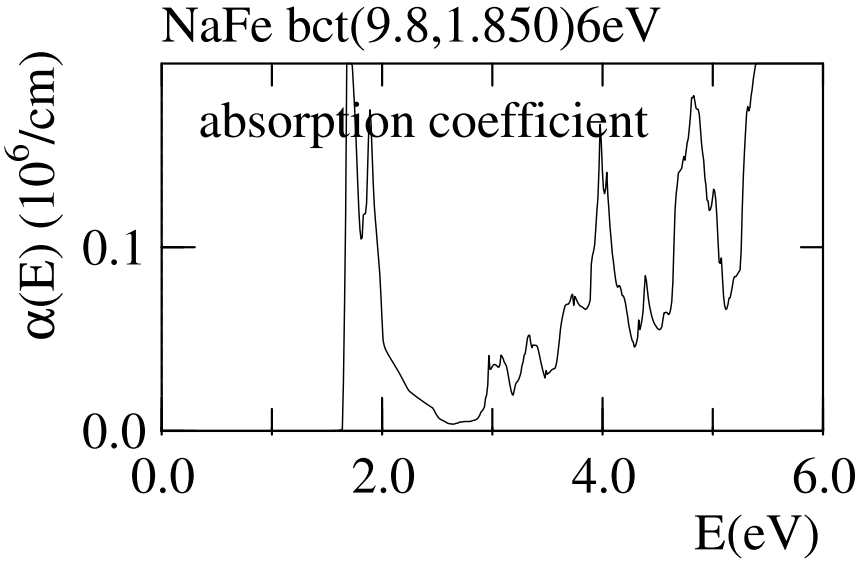
Fe-C	1.85Å
C-N	1.18Å
N-M	1.87Å, 1.97Å

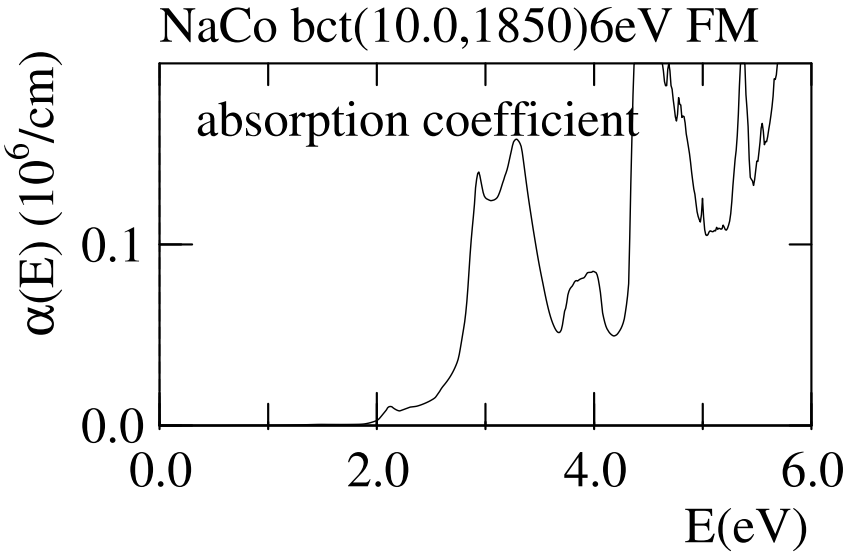
VASP - PAW - optimized structure (NM)

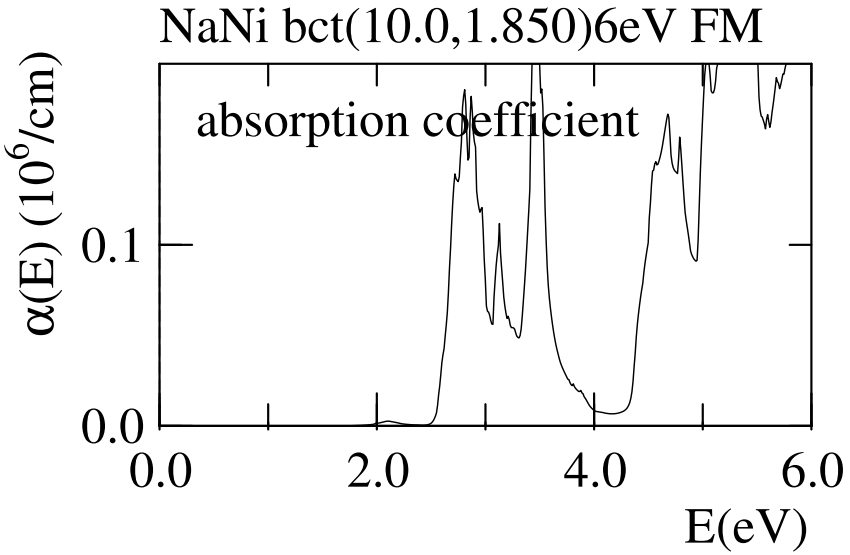
- bct (fcc: $a = 9.854$Å)
- Interatomic distances

Fe-C	1.877Å
C-N	1.174Å
N-Co	1.876Å

Optical absorption NaMFe(CN)$_6$ (M =Fe, Co, Ni) (U_{eff}=6eV)







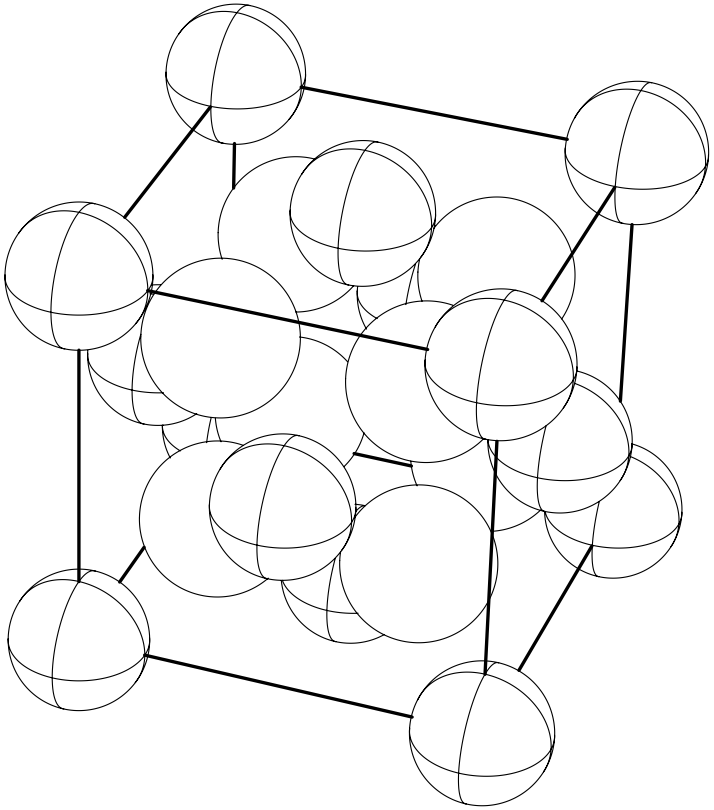
Mg_2Si

Crystal structure:

space group $Fm\bar{3}m$ (No.225);

$a = 6.35$Å

atom	site	position		
Mg	8c	1/4	1/4	1/4
Si	4a	0	0	0



FCC

fluorite (CaF_2) structure

Carrier densities

(Hall measurement)

Electron-doped systems:

Undoped: 8.41×10^{18}/cm^3 (Al)

Bi-I: 7.92×10^{19}/cm^3

Bi=II: 1.38×10^{20}/cm^3

Hole-doped systems:

Ag-I: 7.42×10^{18}/cm^3

Ag-II: 1.50×10^{18}/cm^3

M. Akasaka, T. Iida, et al.

J. Appl. Phys. 104 (2008) 013703.