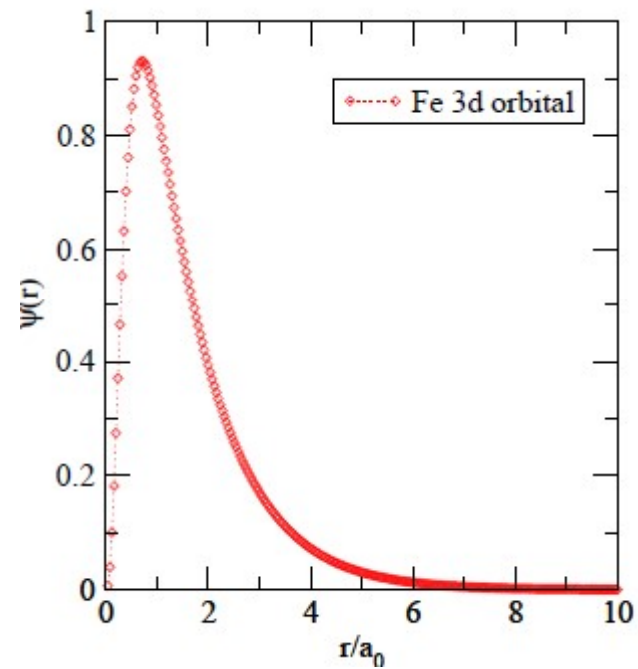


Plane wave method for DFT calculations

Wavefunction (ψ)

- Numerical representation of orbitals / wave functions is necessary for computation.
- It has to be
 - Compact
 - Efficient
 - Accurate
- It should be accurate ($-\nabla^2$) derivatives to calculate K.E.



Recap

- The effective Hamiltonian,

$$[\hat{T}_i + \hat{V}_{ion} + \hat{V}_H + \hat{V}_{XC}]n(r) = En(r)$$

- The density of electrons is represented in terms of wavefunction such as,

$$n(r) = \sum_i^{occ} |\psi_i(r)|^2$$

- We know that the wavefunctions ψ is expressed in a basis set or basis function,

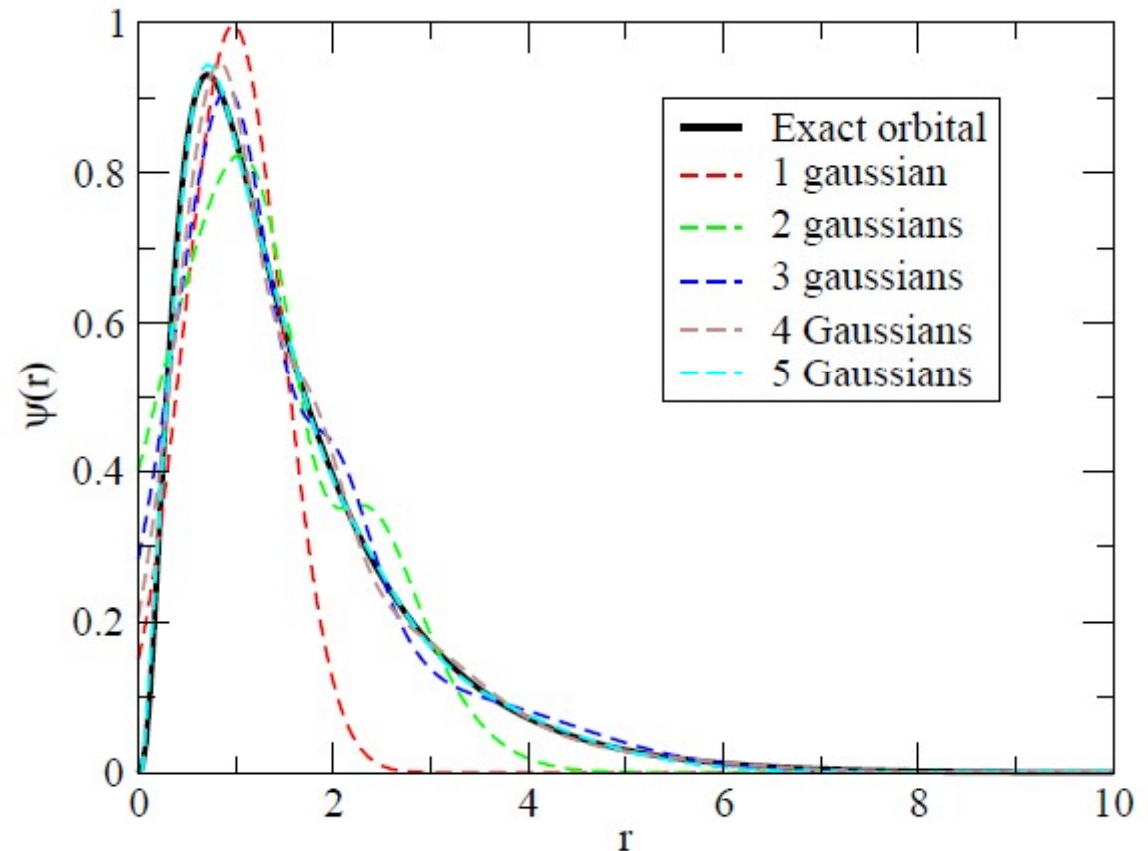
$$\psi = \sum c_i \phi_i$$

- The basis set is expressed in terms of Gaussian function. Hence it is called as Gaussian Basis sets. There are different types of Gaussian functions.
- Gaussian basis sets expression is like

$$\psi_i = \sum_j c_j e^{-\alpha_j r^2} Y_m(\hat{r})$$

Gaussian Basis Set

- Parallel efficient
- Uses different basis sets for molecules and solids
- Expensive to calculate pulay terms such as forces, stresses and force constants
- It consider all electron for calculations



Plane wave basis sets

- Wave vectors (G) are defined in reciprocal lattice vectors which help for periodicity constraint.

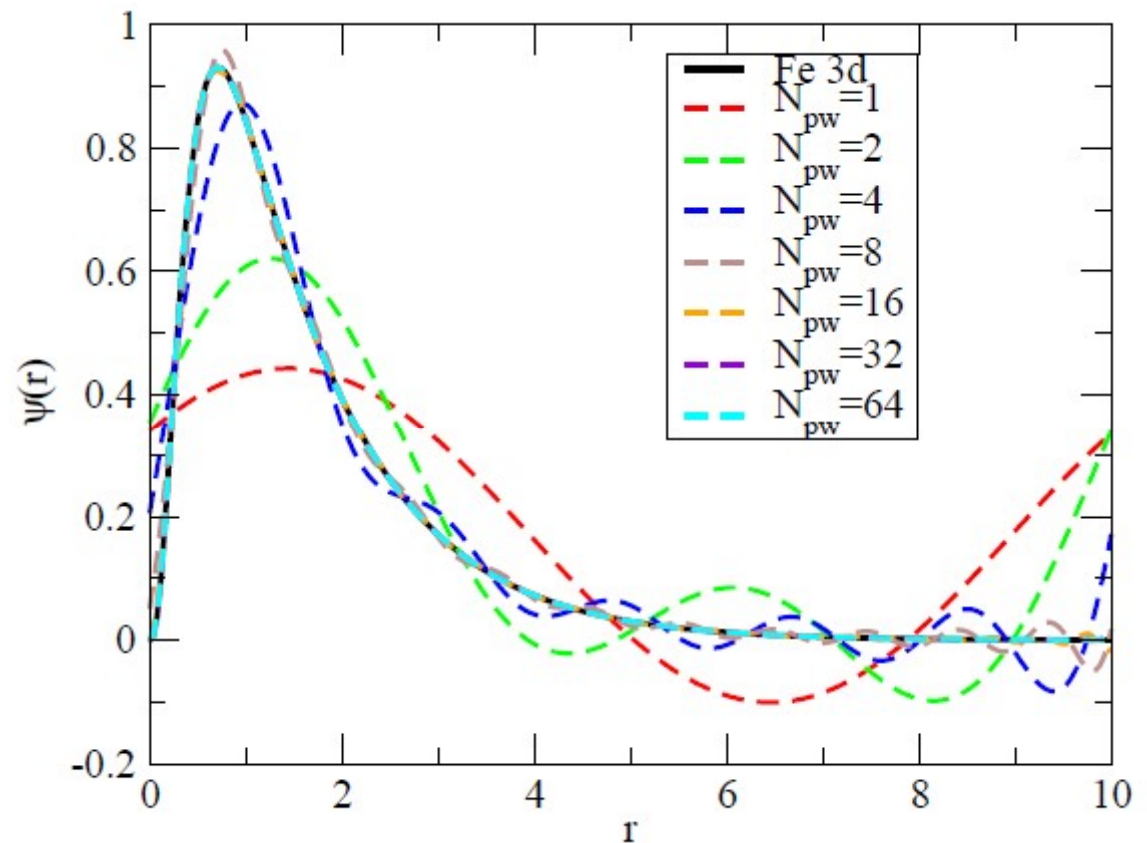
$$\vec{G}_{i_1 i_2 i_3} = \left(i_1 - \frac{N_1}{2} \right) \vec{b}_1 + \left(i_2 - \frac{N_2}{2} \right) \vec{b}_2 + \left(i_3 - \frac{N_3}{2} \right) \vec{b}_3$$

Where b_1 , b_2 and b_3 are reciprocal lattice vectors.

- The plane wave basis sets is,

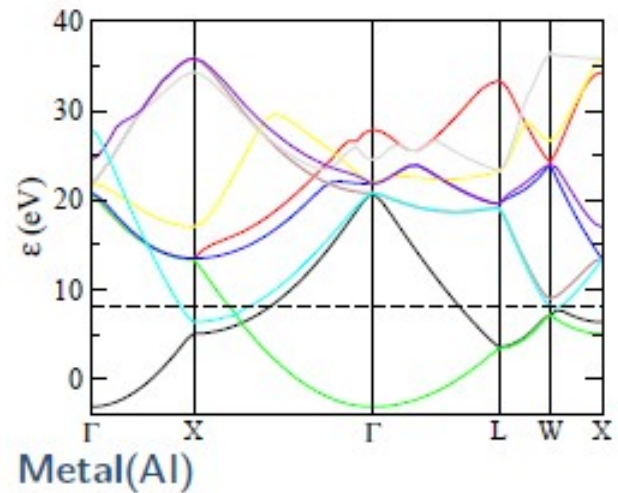
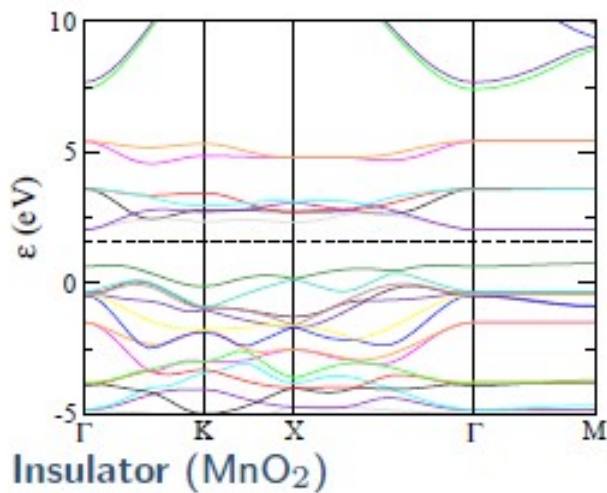
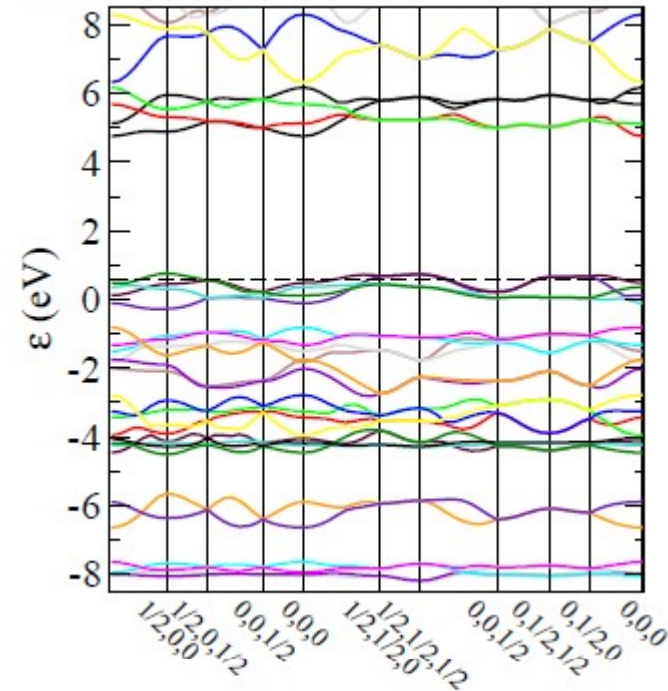
$$\psi_{i,k}(r) = \sum_{|G| < G_{\max}} c_{i,k} G e^{i(k+G).r}$$

- Fast Fourier Transformation (FFT) algorithms used for real and reciprocal space transformations.
- Allow to use more number of atoms.
- Possible to use all electron or only valence electron for calculations.
- Same basis set for molecules and solids.



- Eigen values gives band structure.
- Electrons fill lowest energy state.
- Energy between highest occupied state and lowest unoccupied state gives the Fermi energy

Example: Benzene, Phase III



Band structure related properties

- Optical properties
- Excitation energies
- Electronic transport
- Electron-phonon interactions
- Etc.

Optical Property of SrI₂

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Near optical isotropy in noncubic SrI₂: Density functional calculations

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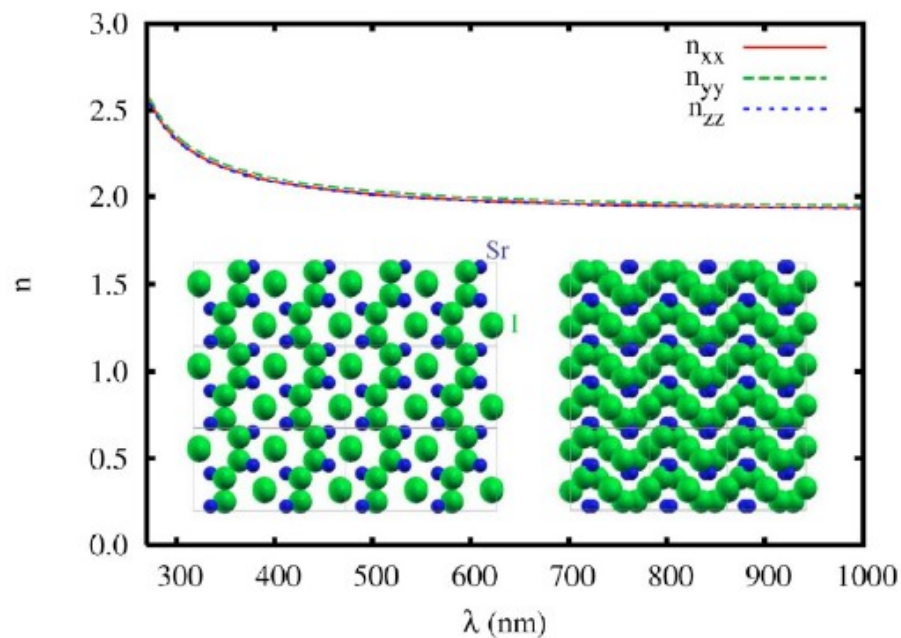


FIG. 4. (Color online) Wavelength dependent refractive index of SrI₂ as obtained with the Engel–Vosko GGA.

Fabrication and Properties of Translucent SrI₂ and Eu:SrI₂ Scintillator Ceramics

Stephen R. Podowitz, Romain M. Gaumé, Wesley T. Hong, Atfal Laouar, and Robert S. Feigelson

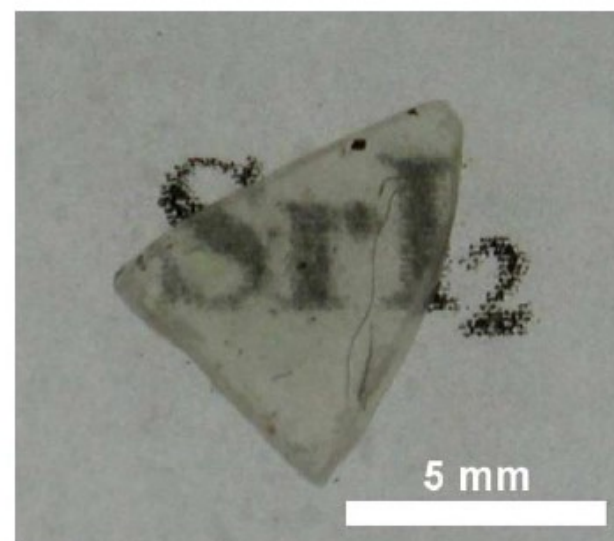


Fig. 5. Translucent ceramic sample of 0.77 mm-thick Eu:SrI₂ backlit.

Magnetic property of Fe₂Ti

Phase	End members	Pearson symbol	ΔE_f	Magnetism
Fe ₂ Ti	(Fe) ₂ (Ti) ₄ (Fe) ₆	<i>hP</i> 16	-30.131	FM ($\mu_B=1.417$)
		<i>hP</i> 16	-29.817	AFM ($\mu_B=0.945$)
		<i>hP</i> 16	-27.134	PM

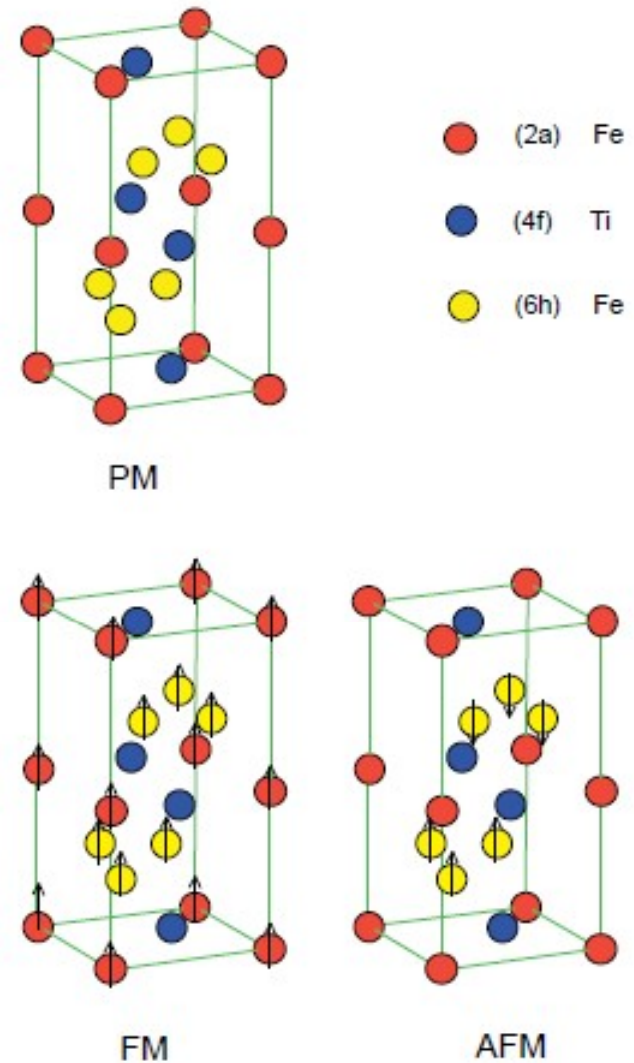


Figure 4.3: Unit cell of Fe₂Ti in C14 Laves crystal structure. PM, FM and AFM indicates para, ferro and antiferro magnetism of Laves phase respectively. Fe atoms occupies (2a) and (6h) sites and Ti atoms occupies (4f) sites.