

First Principle 2017-Fall final Solution

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1. Fe bcc, fcc and hcp structure

(a) using volumn optimization with GGA-PBE potential, the relaxed lattice constant is :

Structure (\AA)	FM a_0	NM a_0
bcc	2.854566	2.7753197
fcc	3.642287	3.4687567
hcp	X	2.47333362 (1.5826)

TABLE I. Results of volumn optimized lattice constant

the value in the parentheses is the c/a ratio. We note that relaxation using vasp cannot get the correct relaxed state for ferromagnetic hcp case.

(b) To get more accurate lattice constant and calculate the bulk modulii, we perturb the lattice constants a little from the relaxed value. By using third order polyfit, and with the following relations, we can get the bulk-modulus B and the minimum a_0 :

$$B = V \frac{\partial^2}{\partial V^2} E$$
$$V = a_0^3$$

Note that in hcp structure the unit-cell volumn is :

$$V = a_0^3 \cdot \left(\frac{\sqrt{3}}{2} \frac{c}{a_0} \right) \quad (1)$$

Following shows the calculated result for FM and NM case with different lattice structure.

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• bcc

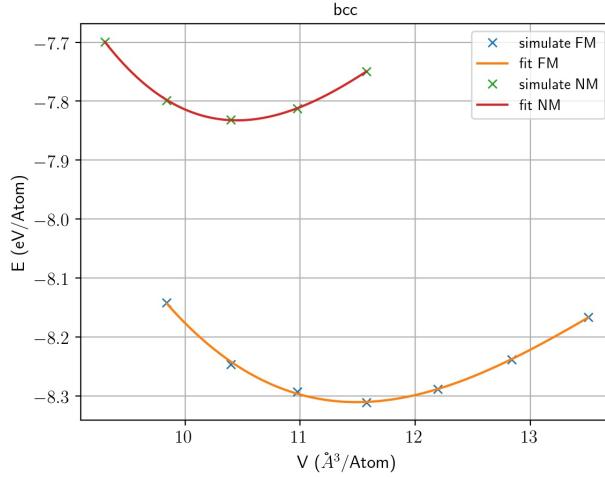


FIG. 1. Fe-bcc E-V

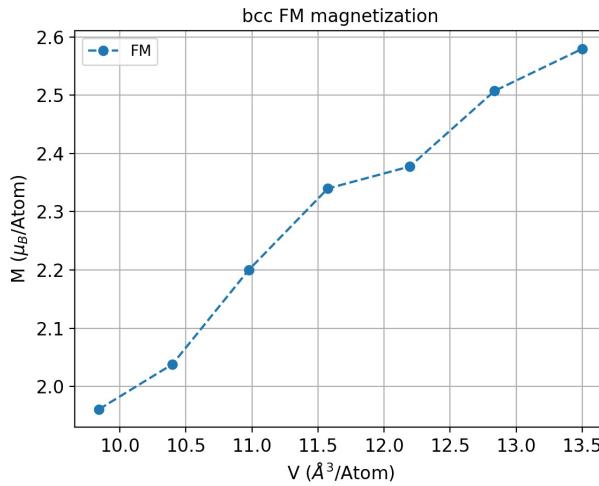


FIG. 2. Fe-bcc M-V

bcc	FM	NM	
a_0	2.84254	2.75474	(Å)
B	183.3448	278.7161	(GPa)

TABLE II. bcc result from fitting with the E-V curve

• fcc

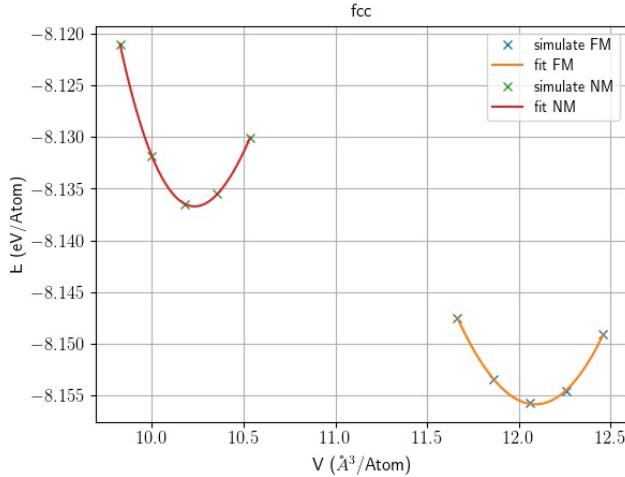


FIG. 3. Fe-fcc E-V

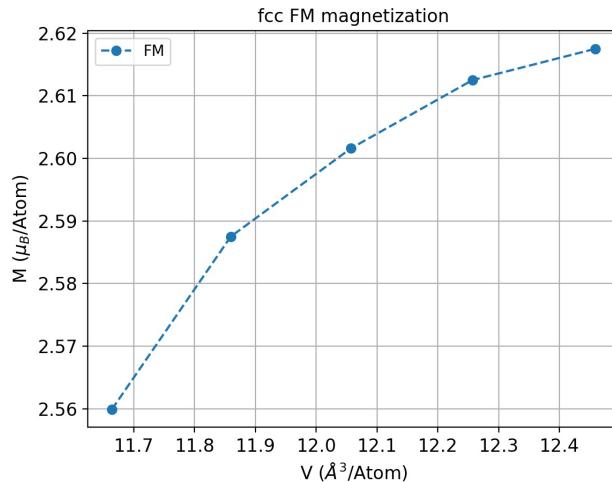


FIG. 4. Fe-fcc M-V

fcc	FM	NM	
a_0	3.64323	3.44638	(Å)
B	185.5447	269.3374	(GPa)

TABLE III. fcc result from fitting with the E-V curve

- hcp

The hcp is calculated with fixed c/a ratio and perturb the lattice constant. Where for FM case $c/a = 1.7320$ and NM case $c/a = 1.5860$

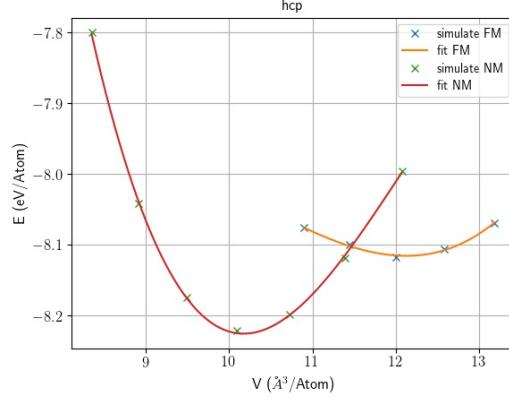


FIG. 5. Fe-hcp E-V

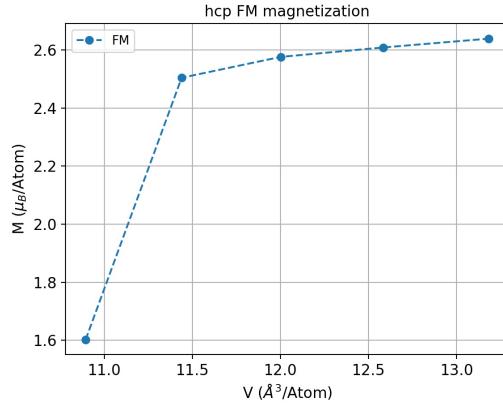


FIG. 6. Fe-hcp M-V

hcp	FM	NM	
a_0	2.52821	2.45619	(Å)
B	135.1516	313.6009	(GPa)

TABLE IV. hcp result from fitting with the E-V curve and fixed c/a

To get the transition pressure from ferro-magnetic bcc to non-magnetic hcp, we use the relation for pressure P :

$$P = -\frac{\partial E}{\partial V} \quad (2)$$

this suggest that the transition happened when the E-V curves for bcc and hcp have the same slopes. following shows the E-V plot and P-V plot for FM-bcc and NM-hcp Fe.

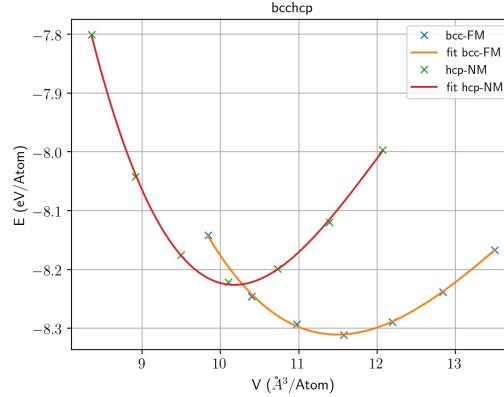


FIG. 7. FM-bcc and NM-hcp E-V

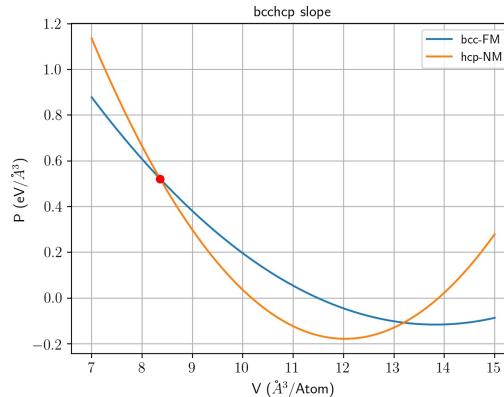


FIG. 8. FM-bcc and NM-hcp P-V

where we find the transition pressure is :

$$P_c = 0.522093(eV/\text{Å}^3) \quad (3)$$

$$= 83.53488(GPa) \quad (4)$$

(c) Finally we list all the calculation results in below:

bcc	FM	NM	
a_0	2.84254	2.75474	(Å)
V_0	11.4839	10.4523	(Å ³ /Atom)
B	183.3448	278.7161	(GPa)
M	2.3312	–	(μ_B /Atom)

fcc	FM	NM	
a_0	3.64323	3.44638	(Å)
V_0	12.0893	10.2336	(Å ³ /Atom)
B	185.5447	269.3374	(GPa)
M	2.6052	–	(μ_B /Atom)

hcp	FM	NM	
a_0	2.52821	2.45619	(Å)
c/a	1.7320	1.5860	
V_0	12.1191	10.1763	(Å ³ /Atom)
B	135.1516	313.6009	(GPa)
M	2.58355	–	(μ_B /Atom)

2. (a) The calculation results of fcc-Au and diamond-Si without spin-orbital coupling.

- Au

Following shows the bands structure, density of state for Au without spin orbital coupling(non-relativistic). The calculation of band structure are consist with previous study [1] and the DOS consist with bulk DOS in [2].

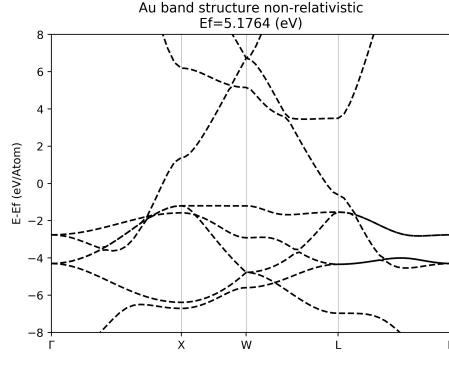


FIG. 9. Au band structure

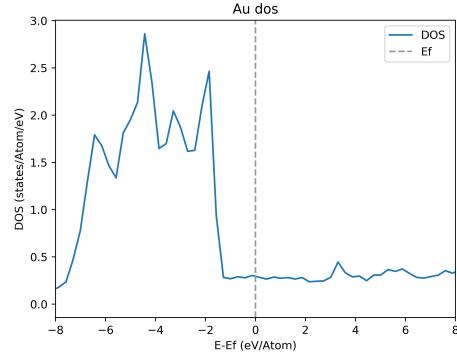


FIG. 10. Au DOS

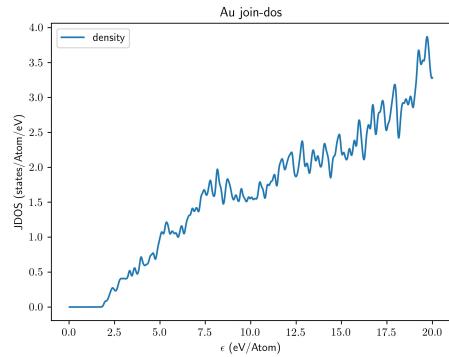


FIG. 11. Au join-DOS

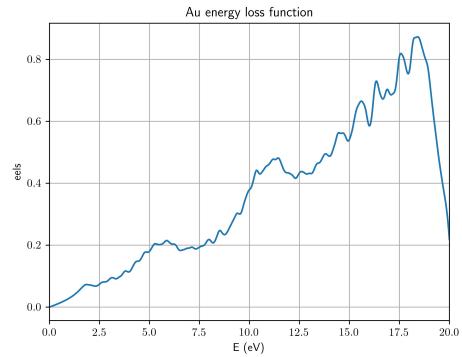


FIG. 12. Au energy loss function

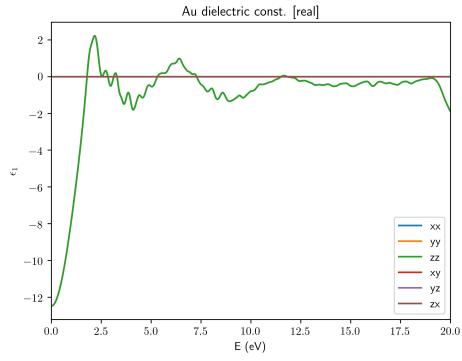


FIG. 13. Au dielectric constant (real)

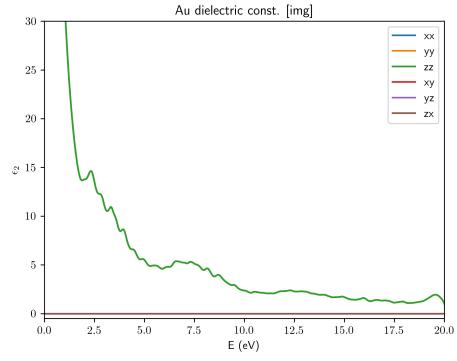


FIG. 14. Au dielectric constant (image)

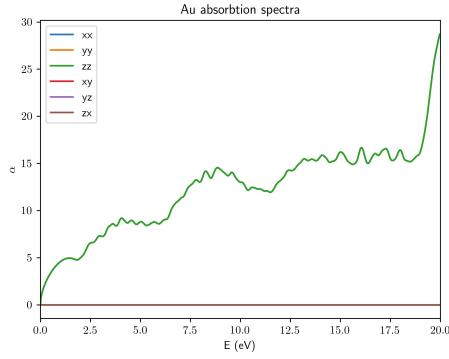


FIG. 15. Au absorption

- Si

Following shows the bands structure, density of states for Si without spin orbital coupling(non-relativistic). The calculation are consist with previous study [3]

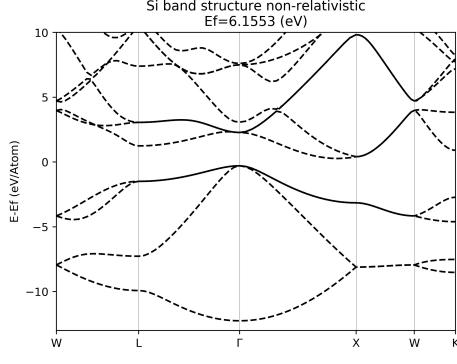


FIG. 16. Si band structure

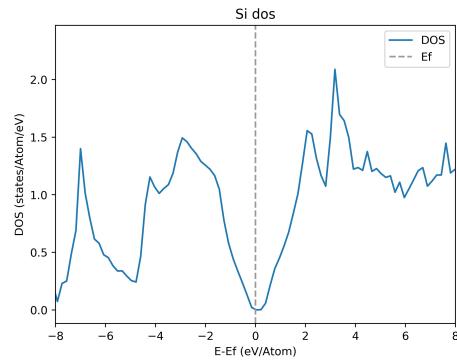


FIG. 17. Si DOS

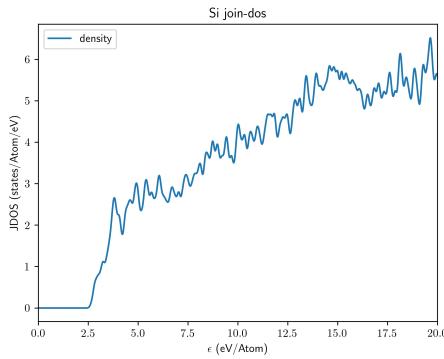


FIG. 18. Si join-DOS

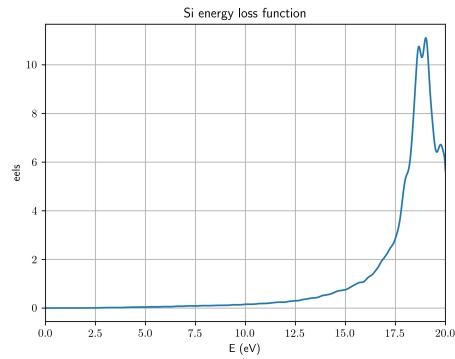


FIG. 19. Si energy loss function

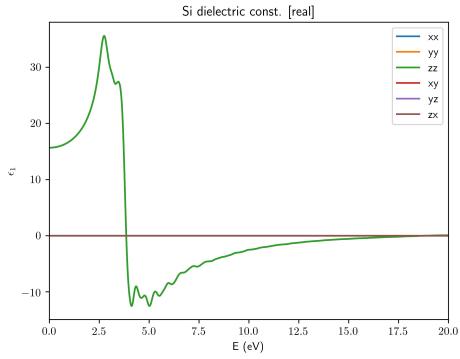


FIG. 20. Si dielectric constant (real)

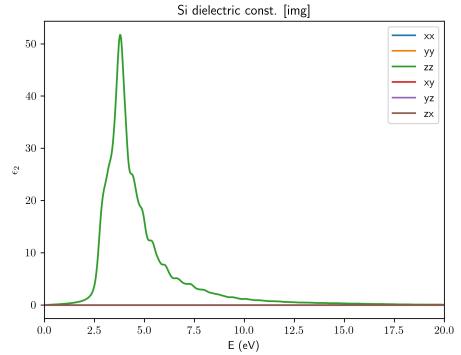


FIG. 21. Si dielectric constant (image)

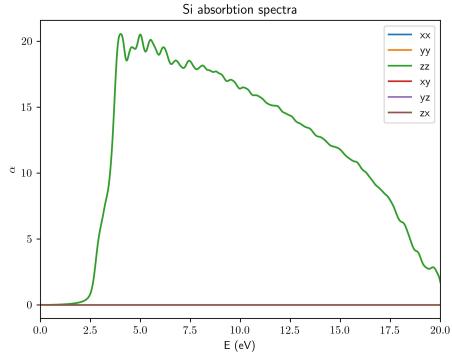


FIG. 22. Si absorption

(b) The calculation results of fcc-Au and diamond-Si with spin-orbital coupling.

- Au

Following shows the bands structure, density of state for Au with spin orbital coupling (relativistic). The calculation of band structure and dos are consist with previous study [1] [4]. Compare with the non-relativistic calculation, we see that the band splitting that due to the spin-orbital coupling can be observe in band structure. Also, The density of states are re-configured when consider the SOC effect.

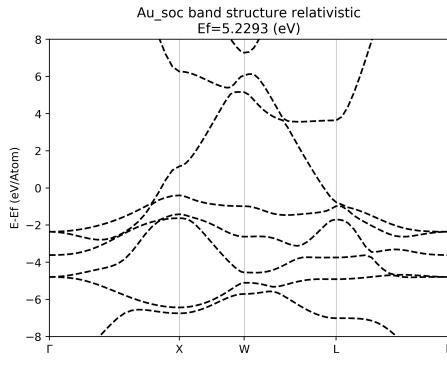


FIG. 23. Au band structure with SOC

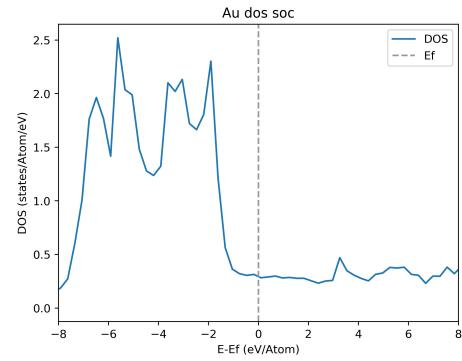


FIG. 24. Au DOS with SOC

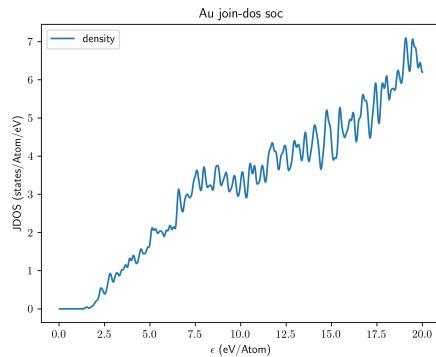


FIG. 25. Au join-DOS with SOC

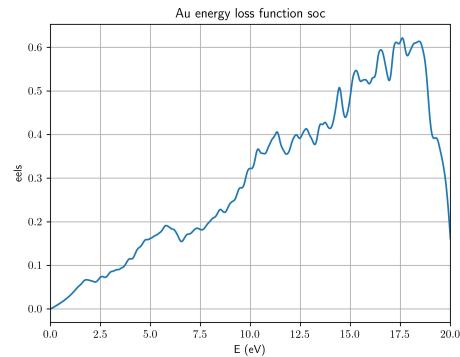


FIG. 26. Au energy loss function with SOC

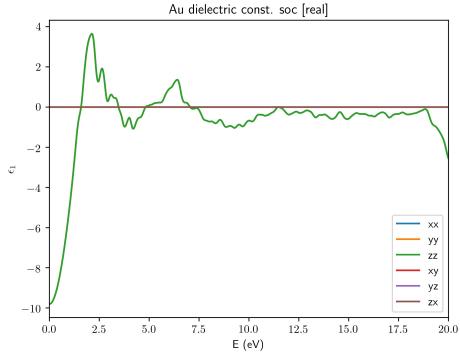


FIG. 27. Au dielectric constant (real) with SOC

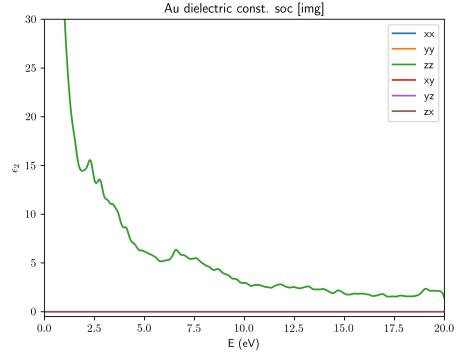


FIG. 28. Au dielectric constant (image) with SOC

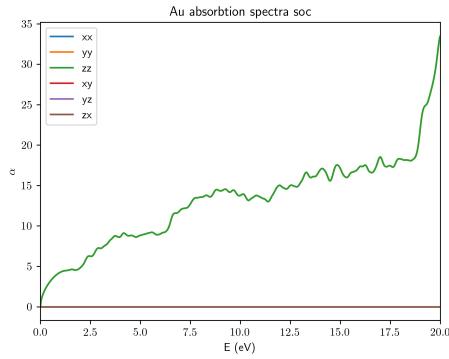


FIG. 29. Au absorption with SOC

- Si

Following shows the bands structure, density of states for Si with spin orbital coupling (relativistic). Compare to Au, with the effect of spin-orbital coupling, the calculation results of Si doesn't differ much with non-relativistic calculation.

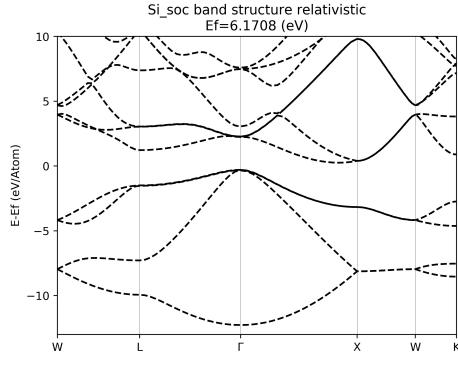


FIG. 30. Si band structure with SOC

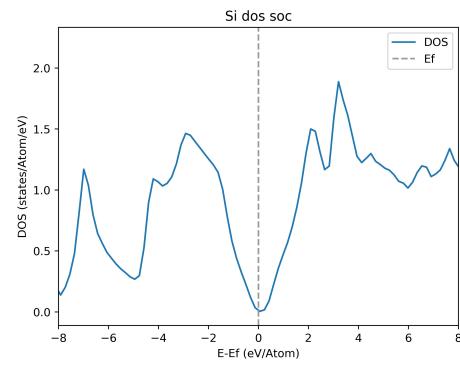


FIG. 31. Si DOS with SOC

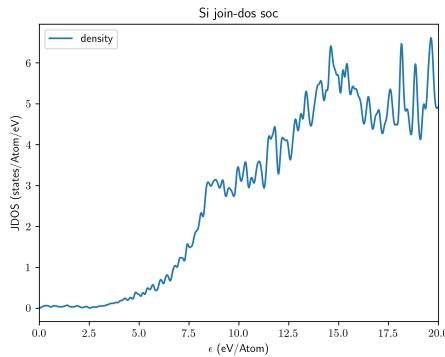


FIG. 32. Si join-DOS with SOC

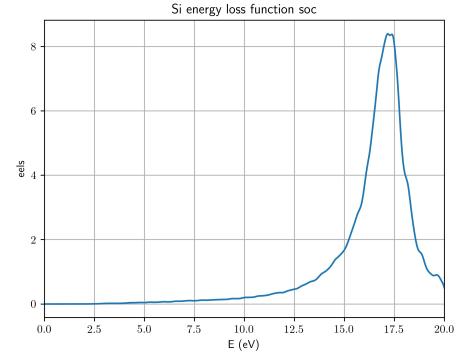


FIG. 33. Si energy loss function with SOC

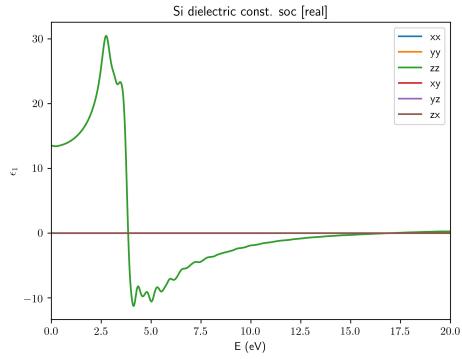


FIG. 34. Si dielectric constant (real) with SOC

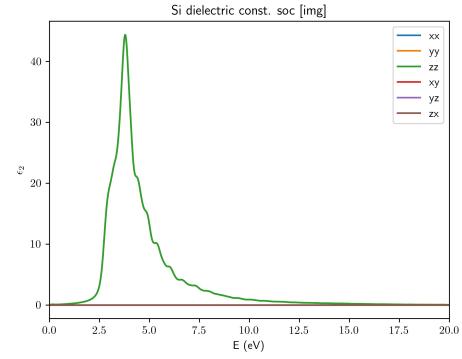


FIG. 35. Si dielectric constant (image) with SOC

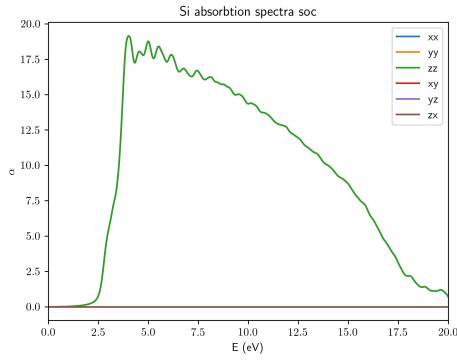


FIG. 36. Si absorption with SOC

3. GGA-PBE calculation of Si and it's thermal dynamic properties.

- (a) Using GGA-PBE potential with structure optimization, the relaxed lattice constant is calculated as :

$$a_0 = 5.3945 \text{ \AA} \quad (5)$$

By self-consistent calculation, the band structure is calculated. Show as following:

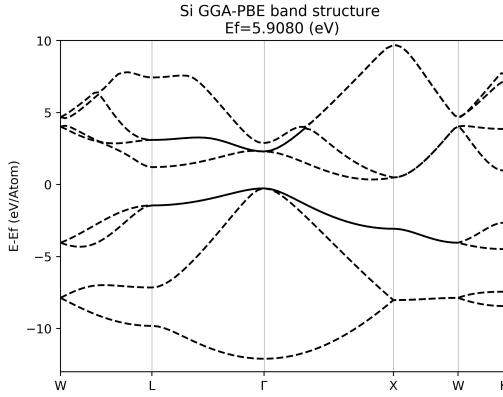


FIG. 37. Si band-structure calculated with GGA-PBE potential

The calculated band structure consist with previous work [3].

- (b) For phonon dispersion. The following results are calculated with the relaxed lattice constant with $2 \times 2 \times 2$ super cell and $3 \times 3 \times 3$ super cell respectively.

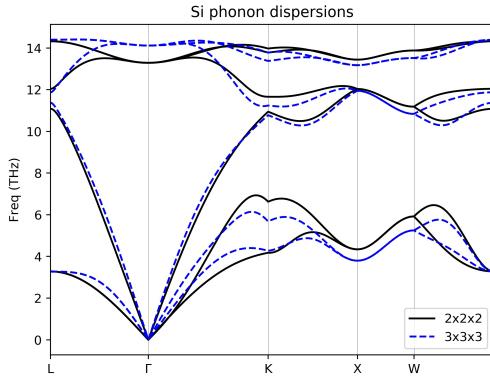


FIG. 38. Si phonon dispersion calculated with GGA-PBE potential

(c) Following shows the thermal dynamic properties of internal energy, free energy, entropy and specific heat results with $2\times 2\times 2$ super cell and $3\times 3\times 3$ super cell respectively.

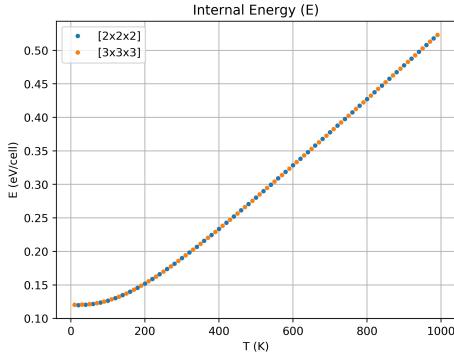


FIG. 39. Si internal energy

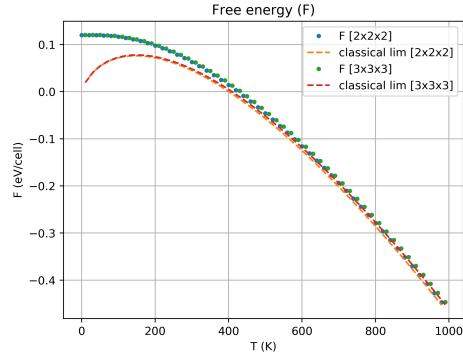


FIG. 40. Si free energy

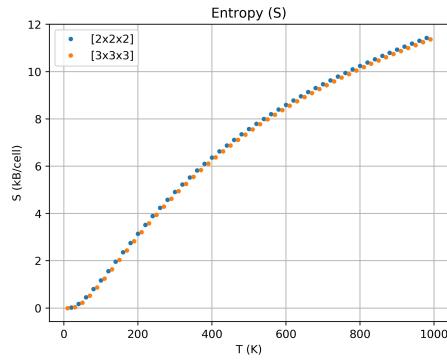


FIG. 41. Si entropy

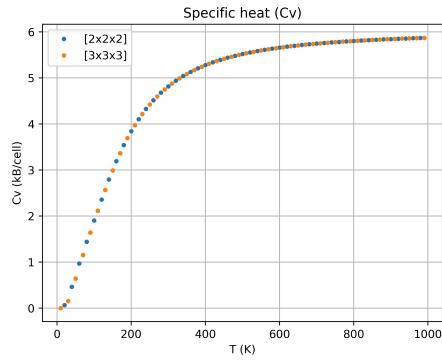


FIG. 42. Si specific heat

4. Compute coupling constant J and transition temperature for Mn bcc.

(a) for lattice constant $a = 2.89 \text{ \AA}$, the calculated energy for FM and AM states:

$$E_{FM} = -17.5978200 \text{ (eV)}$$

$$E_{AM} = -17.4800880 \text{ (eV)}$$

(b) The coupling constant J can be calculated with results in (a) with relation :

$$E_{FM} = E_{PM} + 8J$$

$$E_{AF} = E_{PM} - 8J$$

$$\begin{aligned} J &= (E_{FM} - E_{AF}) / 16 \\ &= -0.0073583 \text{ (eV)} \end{aligned}$$

Using mean field approximation we can calculate the transition point where $z = 8$ is the number of neighbors and $S = \frac{1}{2}$ is the spin moment:

$$\begin{aligned} k_B T_c &= \frac{zJ}{3} \\ T_c &= \frac{8J}{3k_B} \\ &\approx 227.7053K \end{aligned}$$

(c) We refer to [5], which reported the magnetization of ferromagnetic bcc-Mn for different lattice constant. Compare with calculation result with $a = 2.89\text{\AA}$:

$$\begin{aligned} m_{ref} &= 0.97(\mu_B) \\ m_{cal} &= 1.0198(\mu_B) \end{aligned}$$

We see that the result are consist with calculation done in[5]

- [1] M. G. Ramchandani, Journal of Physics C: Solid State Physics **3**, S1 (1970).
- [2] S. V. Boriskina, J. K. Tong, Y. Huang, J. Zhou, V. Chiloyan, and G. Chen, Photonics **2**, 659 (2015).
- [3] X. Liu, L. Liu, X. Wu, and P. K. Chu, Physics Letters A **379**, 1384 (2015).
- [4] S. Kupratakuln, Journal of Physics C: Solid State Physics **3**, S109 (1970).
- [5] G. Fuster, N. E. Brener, J. Callaway, J. L. Fry, Y. Z. Zhao, and D. A. Papaconstantopoulos, Phys. Rev. B **38**, 423 (1988).