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Computation of MOKE spectra

UNi_2Si_2, AuMnX (X = In, Sn, Sb), and Co_2FeSi

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Outline

- ASW scheme
- optical conductivity tensor elements
- UNi_2Si_2
- Heusler alloys

ASW

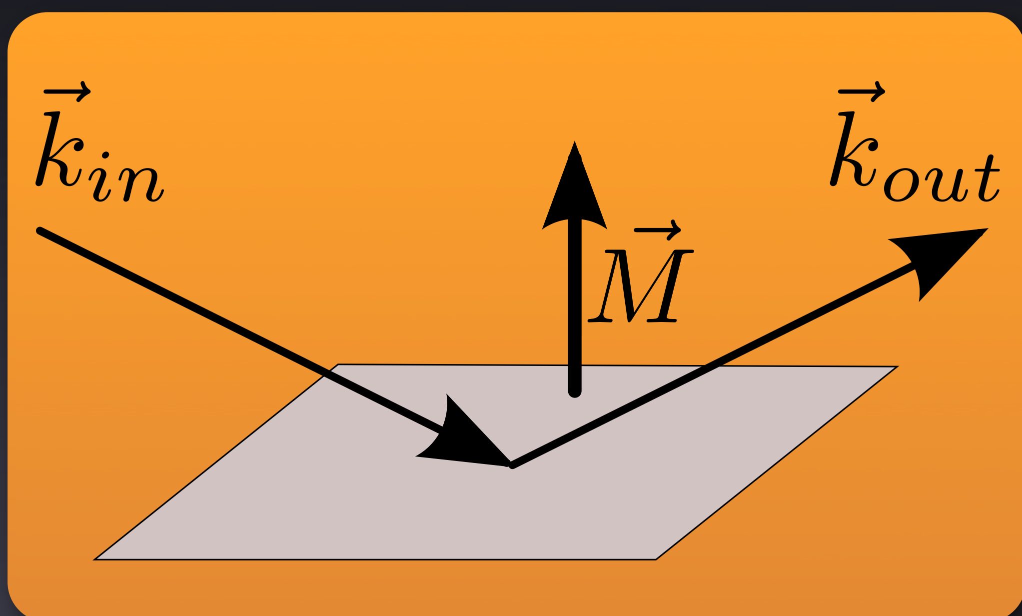
Augmented Spherical Waves

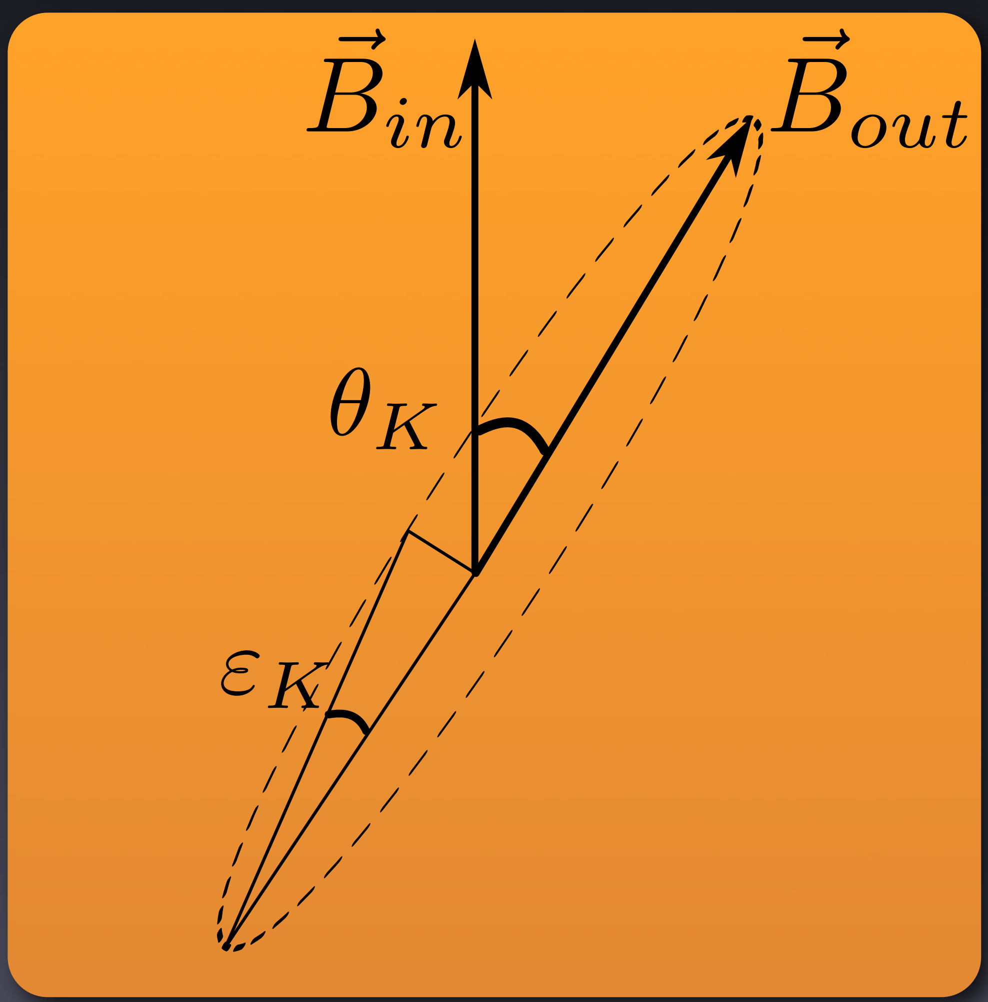
- descendant of LMTO
- using Hankel functions in the interstitial
- fully relativistic LSDA
- (GGA, LDA+U, and non-collinear magnetism)

Williams, Kübler, PRB 19, 1979

p-MOKE

polar Magneto-Optical Kerr Effect





$$\theta_k + i\varepsilon_K = \frac{-\sigma_{xy}}{\sigma_{xx}\sqrt{1 + i\left(\frac{4\pi}{\omega}\right)\sigma_{xx}}}$$

Oppeneer, Handbook of Magnetic Materials, vol. 13, 2001

Optical conductivity

interband contribution

$$\sigma_{xy}(\omega) = \frac{ie^2}{m^2\hbar}\sum_{\mathbf{k}}\sum_{l\sigma_1}^{occ}\sum_{n\sigma_2}^{unocc}\frac{1}{\omega_{n\sigma_2\sigma_1}(\mathbf{k})}\left(\frac{\Pi^x_{l\sigma_1 n\sigma_2}\Pi^y_{n\sigma_2 l\sigma_1}}{\omega - \omega_{n\sigma_2 l\sigma_1}(\mathbf{k}) + i\delta} + \frac{\left(\Pi^x_{l\sigma_1 n\sigma_2}\Pi^y_{n\sigma_2 l\sigma_1}\right)^*}{\omega + \omega_{n\sigma_2 l\sigma_1}(\mathbf{k}) + i\delta}\right)$$

$$\sigma_{xx}(\omega) = \frac{ie^2}{m^2\hbar}\sum_{\mathbf{k}}\sum_{l\sigma_1}^{occ}\sum_{n\sigma_2}^{unocc}\frac{1}{\omega_{n\sigma_2\sigma_1}(\mathbf{k})}\left(\frac{\left|\Pi^x_{l\sigma_1 n\sigma_2}\right|^2}{\omega - \omega_{n\sigma_2 l\sigma_1}(\mathbf{k}) + i\delta} + \frac{\left|\Pi^x_{l\sigma_1 n\sigma_2}\right|^2}{\omega + \omega_{n\sigma_2 l\sigma_1}(\mathbf{k}) + i\delta}\right)$$

$$\Pi_{n\sigma_2 l\sigma_1}(\mathbf{k}) = \int \psi^*_{nk\sigma_2}(\mathbf{r})\left[\mathbf{p} + \left(\frac{\hbar}{4mc^2}\right)[\boldsymbol{\sigma}\times\boldsymbol{\nabla}V(\mathbf{r})]\right]\psi_{lk\sigma_1}(\mathbf{r})\,d\mathbf{r}$$

C.S. Wang and J. Callaway, PRB 9, 1974

Oppeneer et al., PRB 45, 1992

Optical conductivity

intraband contribution

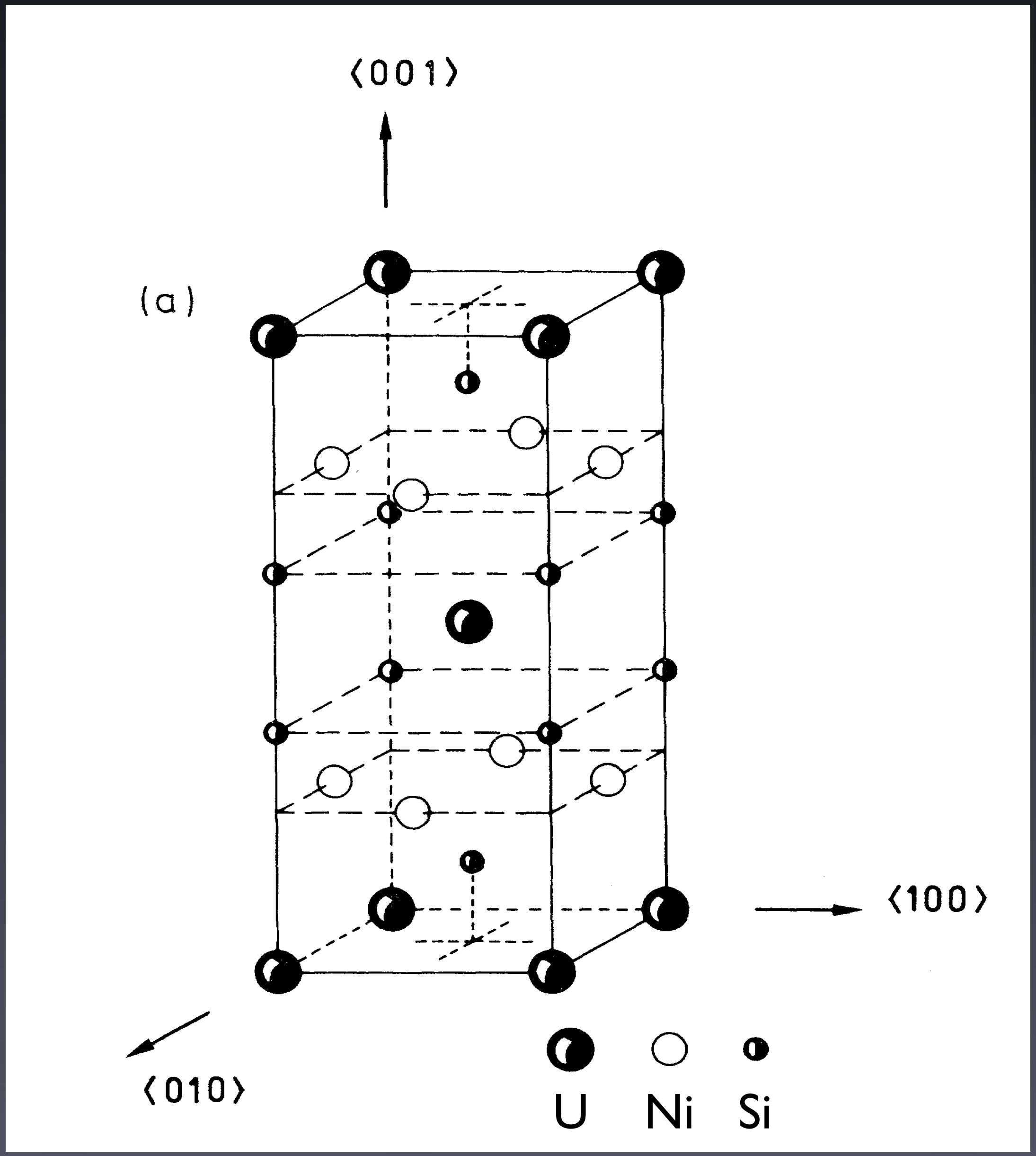
$$\sigma_D(\omega) = \frac{\sigma_0}{1 - i\,\omega\,\tau_D}$$

Paul Drude (1905)

Oppeneer et al., PRB 45, 1992

UNi_2Si_2

structure



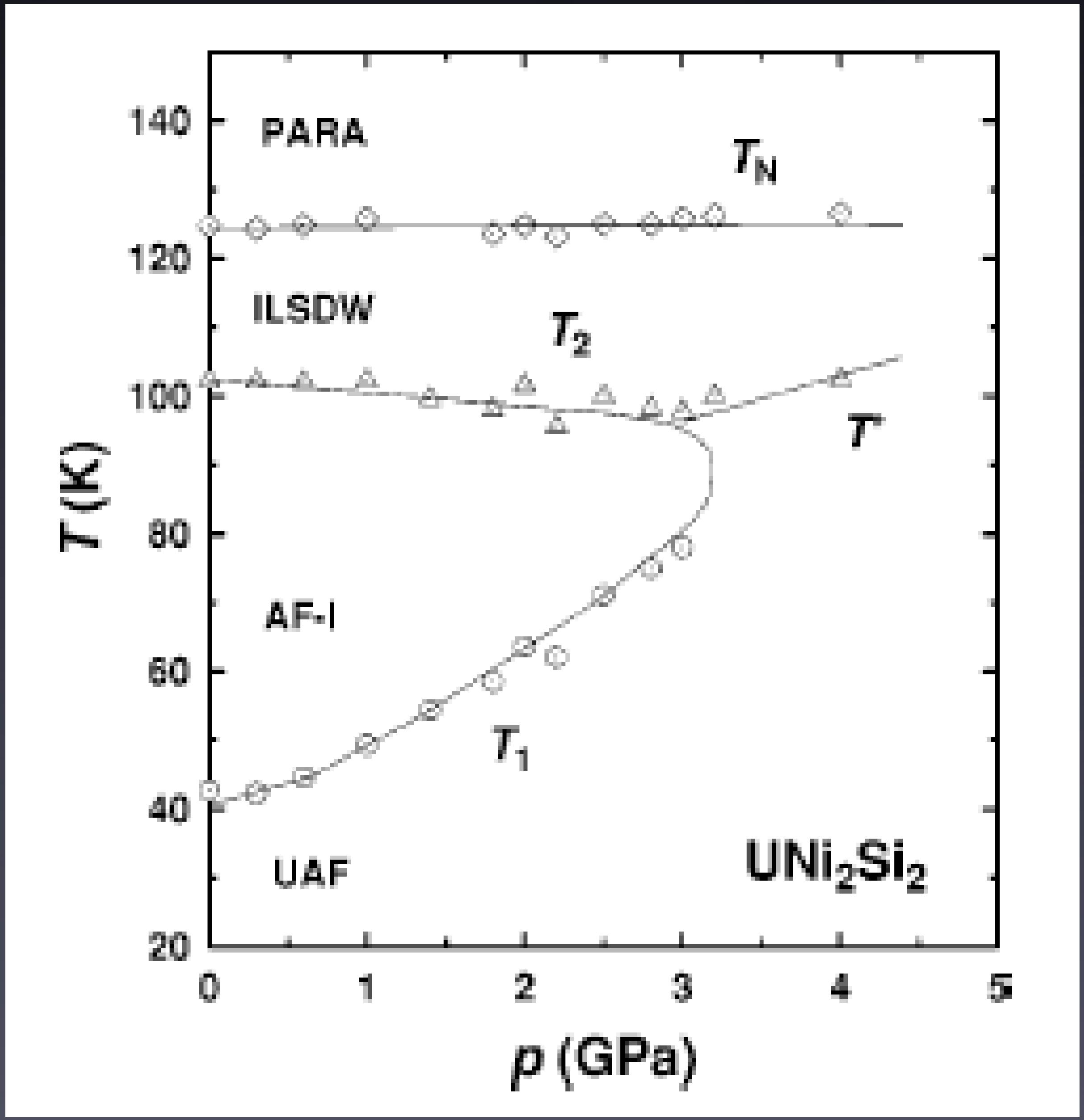
I4 / mmm

	UNi_2Si_2
a (Å)	3.99
c / a	2.388
m^U_{tot} (μ_B)	1.6

Honda et al., PRB 64, 2001

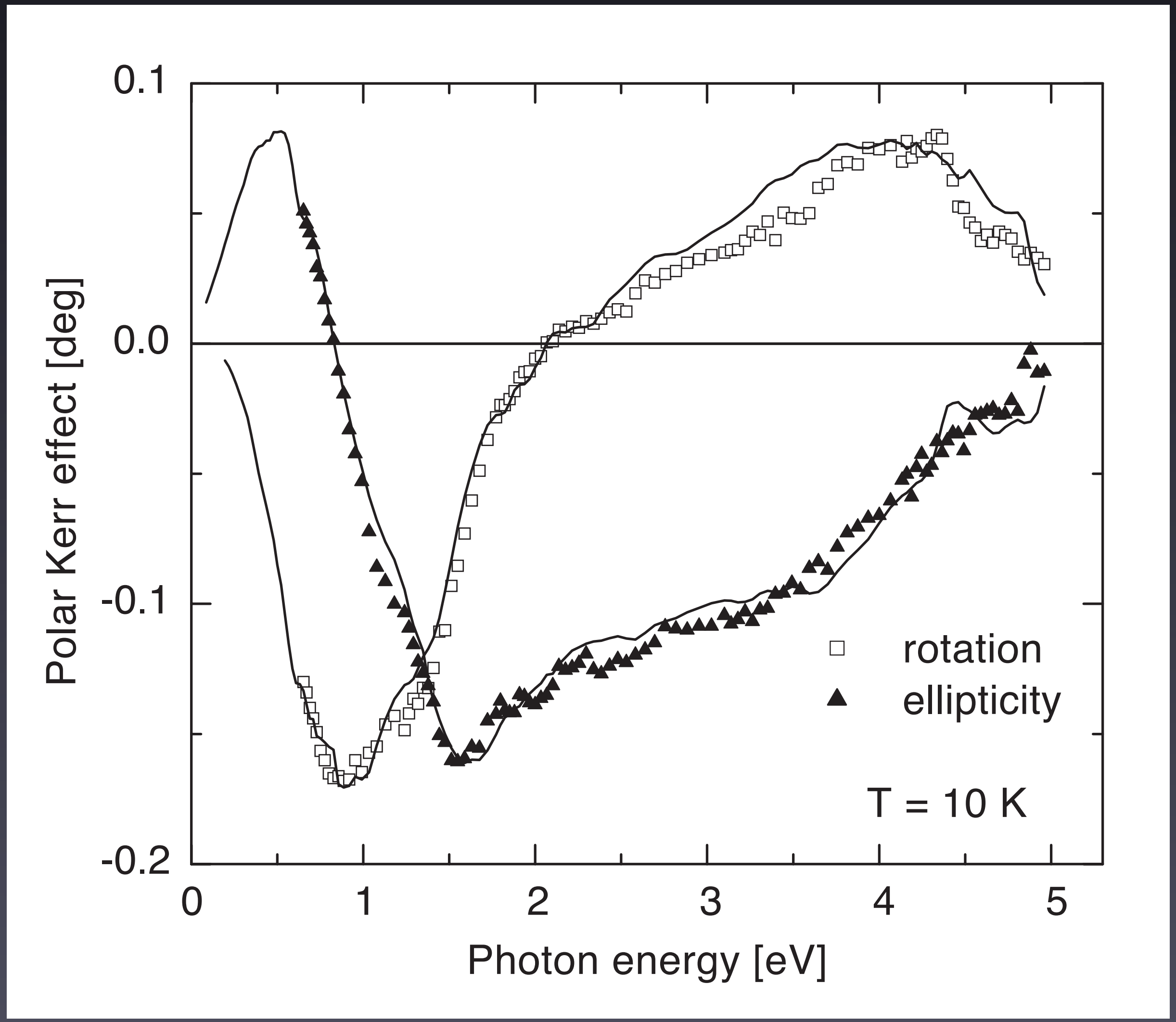
UNi_2Si_2

experimental results



Honda et al., PRB 64, 2001

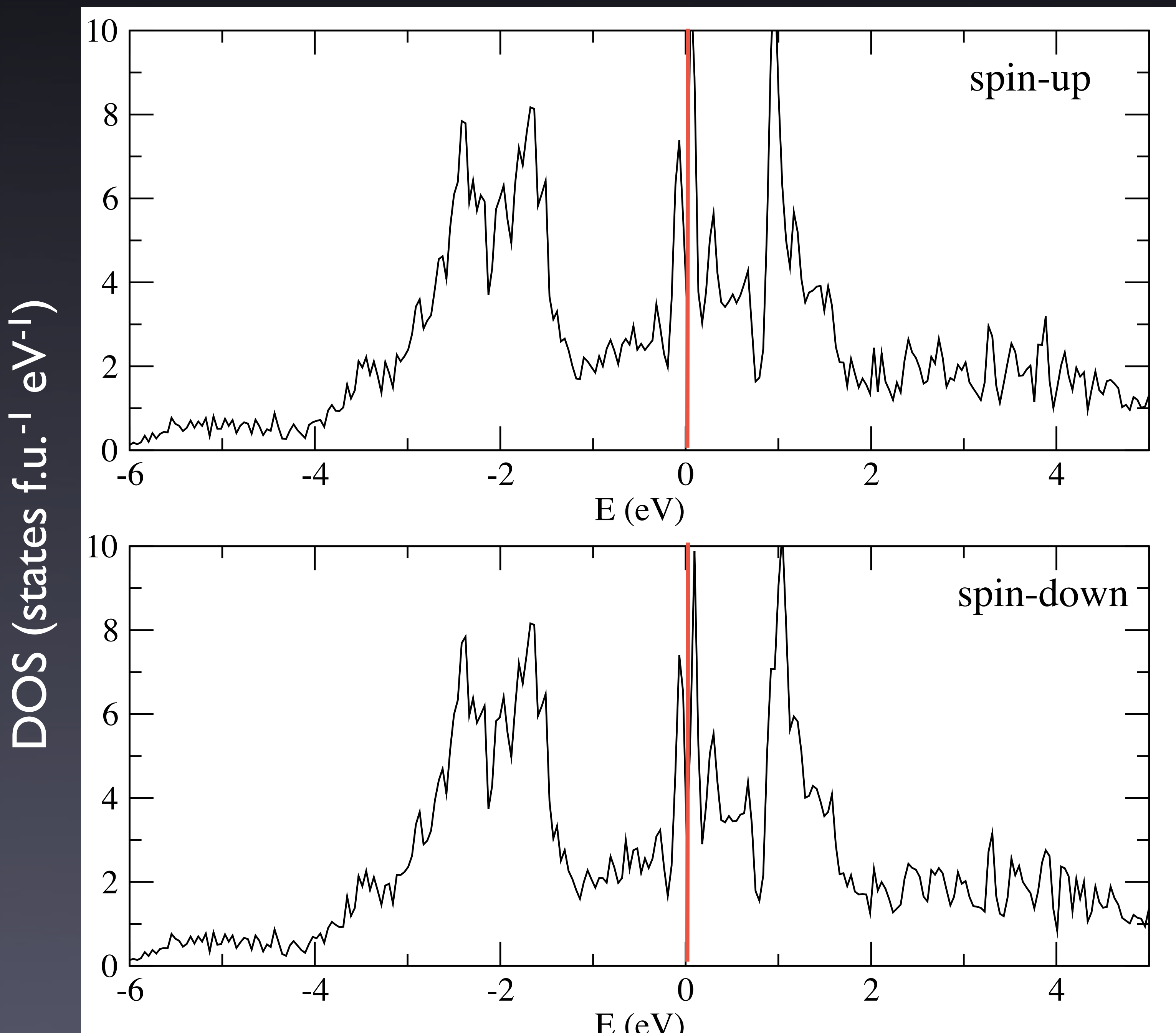
MOKE || c-axis, T = 10K, B = 4T



Kucera et al., JMMM 290-291, 2005

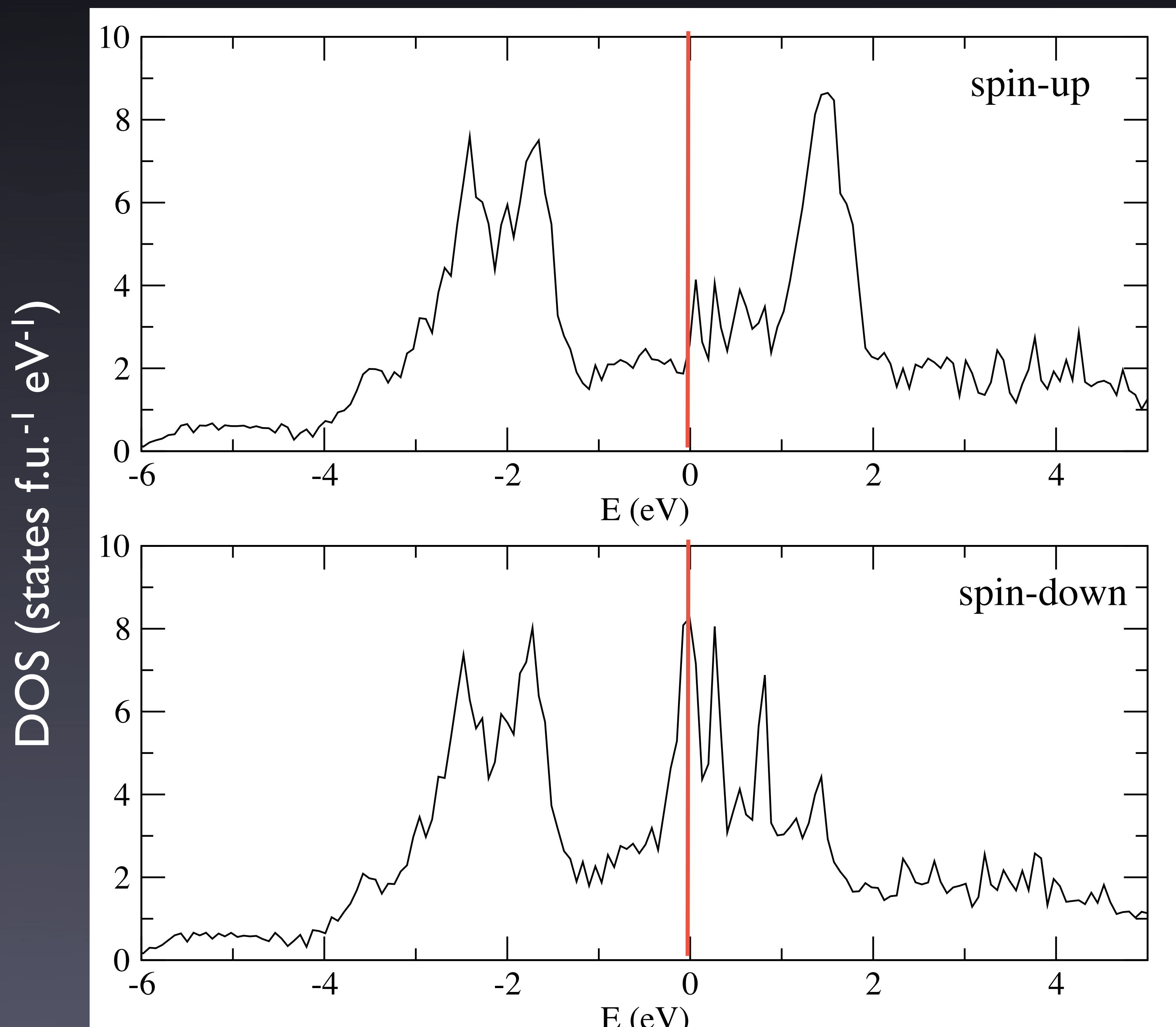
UNi_2Si_2

input: experimental parameters



a_{exp}(Å)	3.974
z / a	0.393
$m_S^U(\mu_B)$	0.16
$m_{tot}^U(\mu_B)$	-0.01
$m/f.u.(\mu_B)$	-0.01

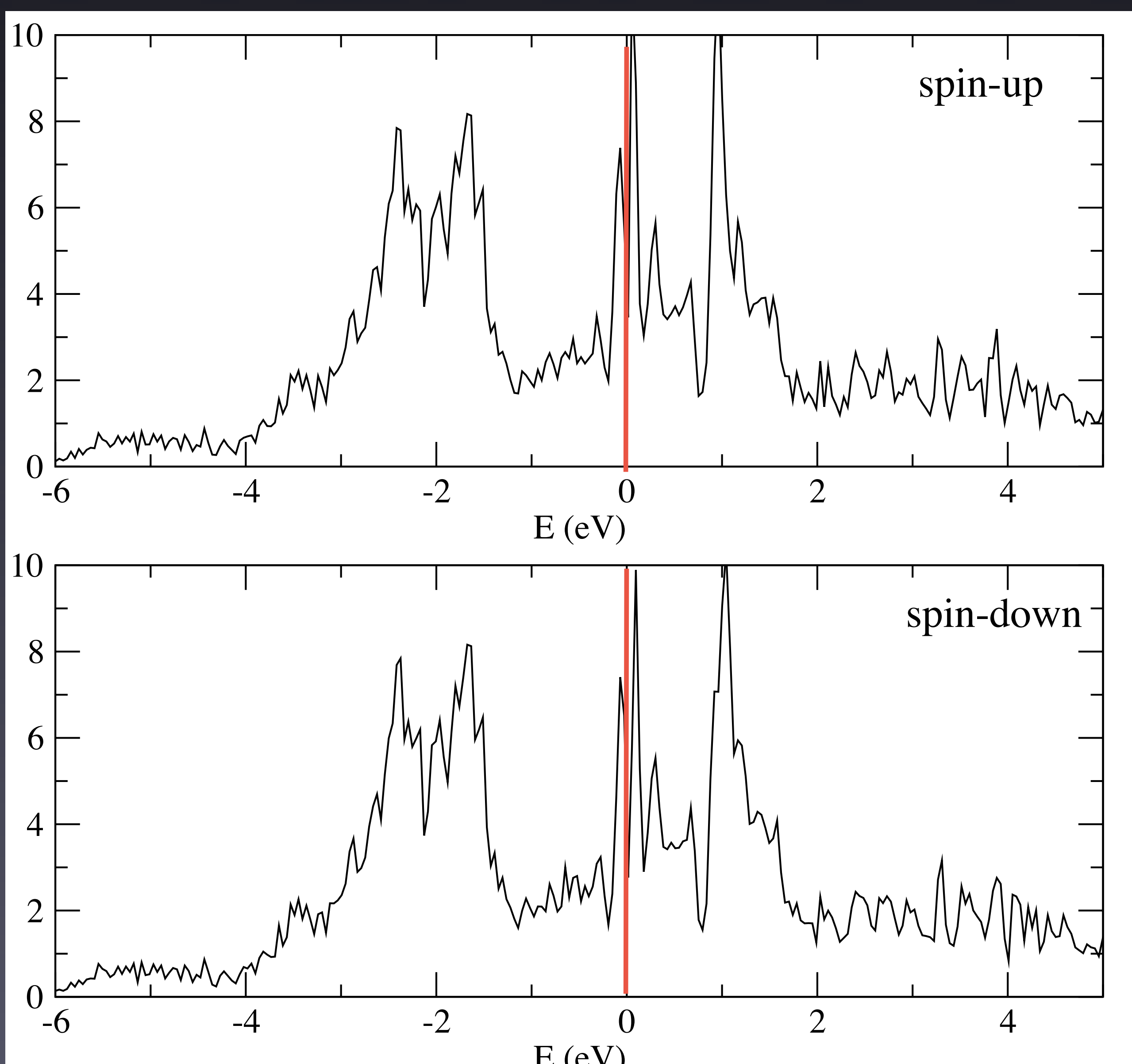
UNi_2Si_2

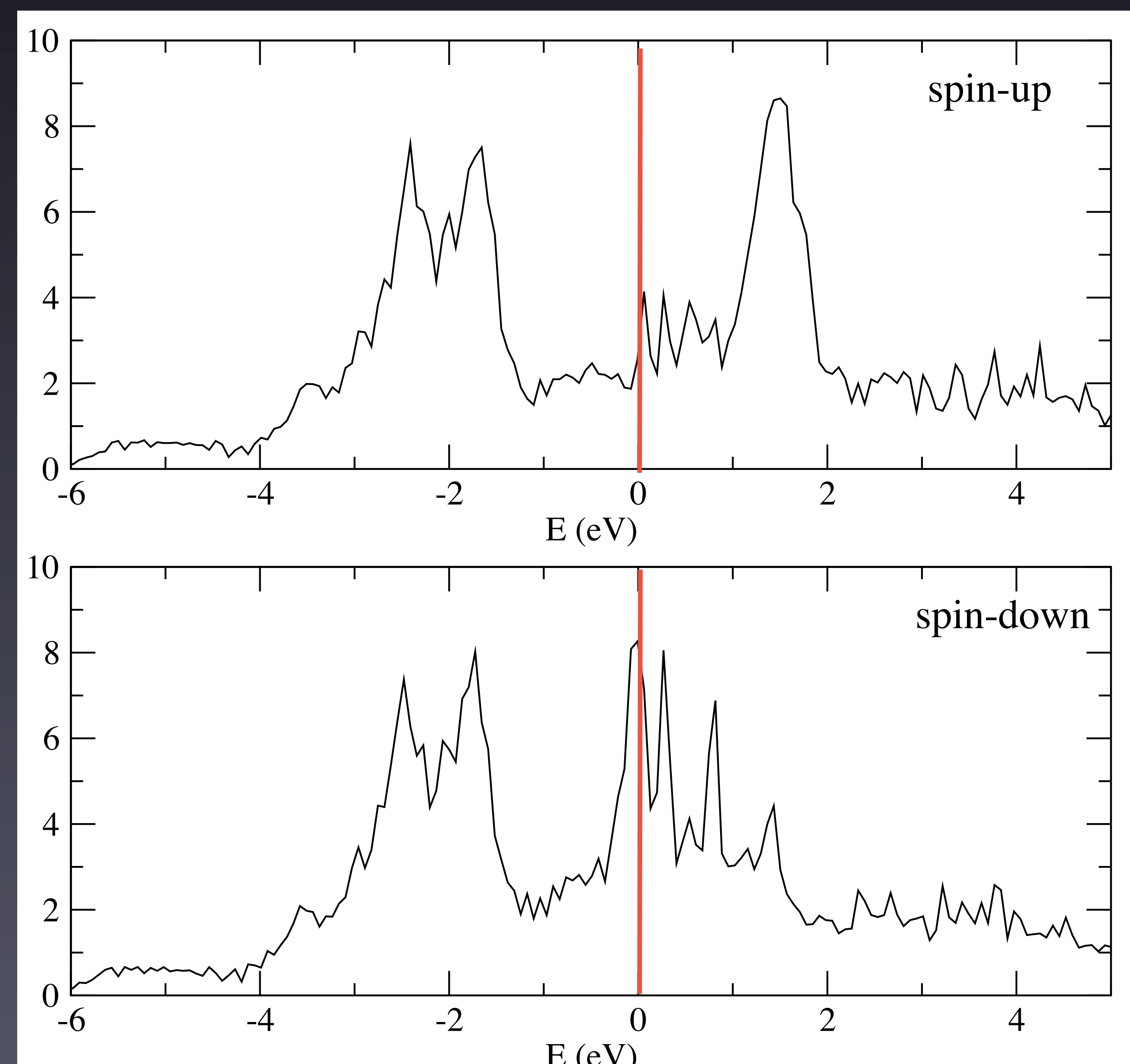


a (Å)	3.955
z / a	0.393
$m_S^U(\mu_B)$	1.65
$m_{tot}^U(\mu_B)$	0.79
$m/f.u.(\mu_B)$	0.66

UNi_2Si_2

comparison

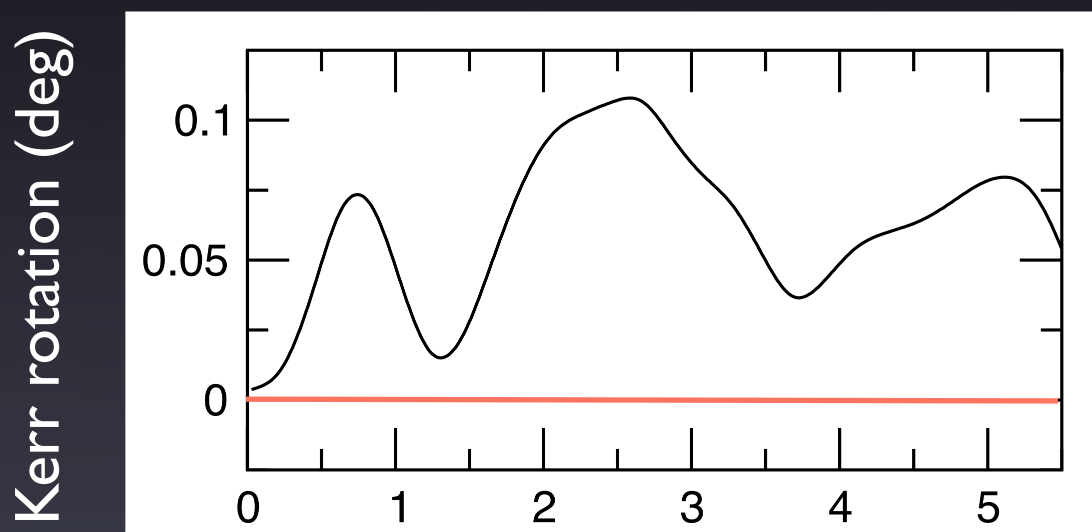


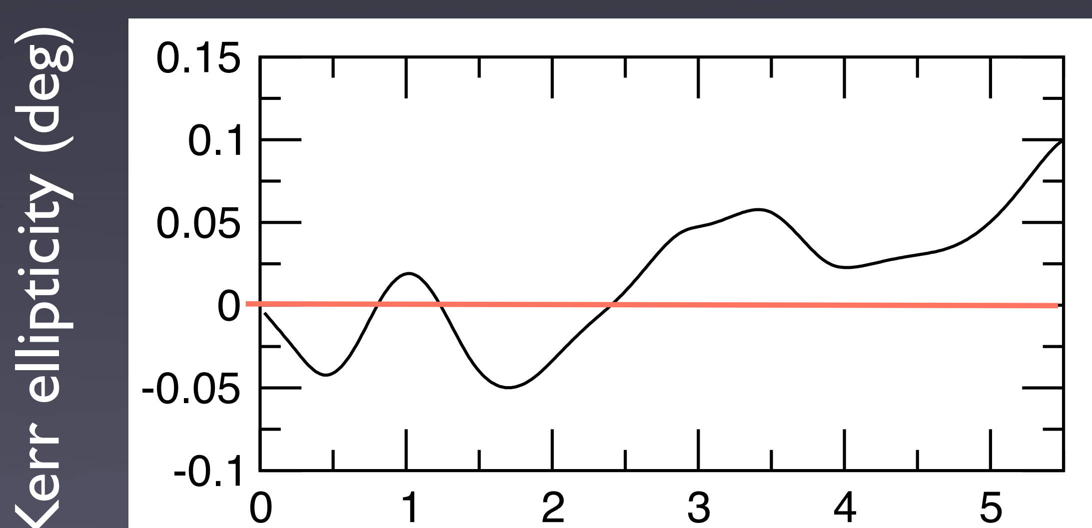


UNi_2Si_2

computed MOKE

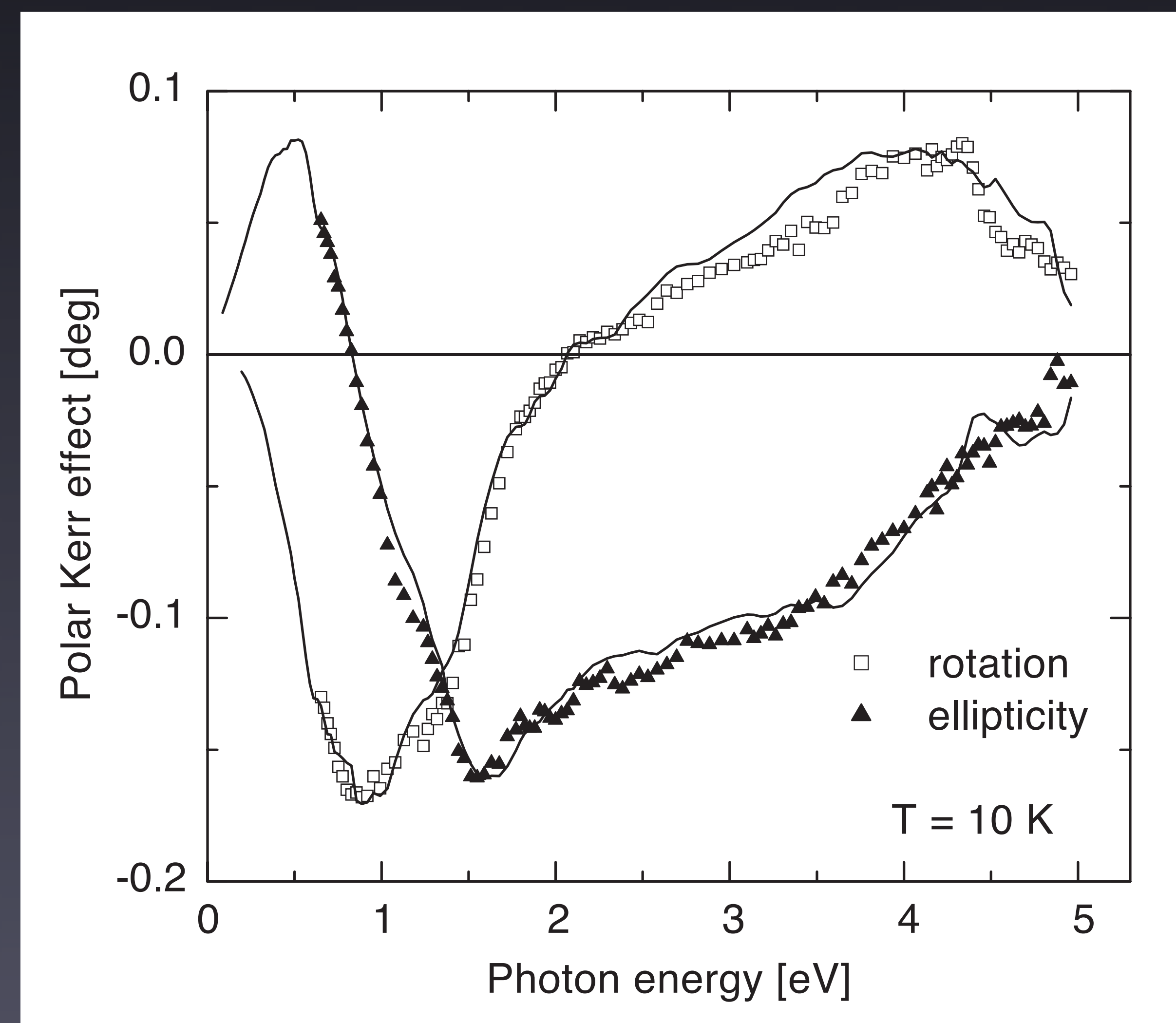
a_{exp} = 3.974 Å





Energy (eV)

MOKE || c-axis, T = 10K, B = 4T

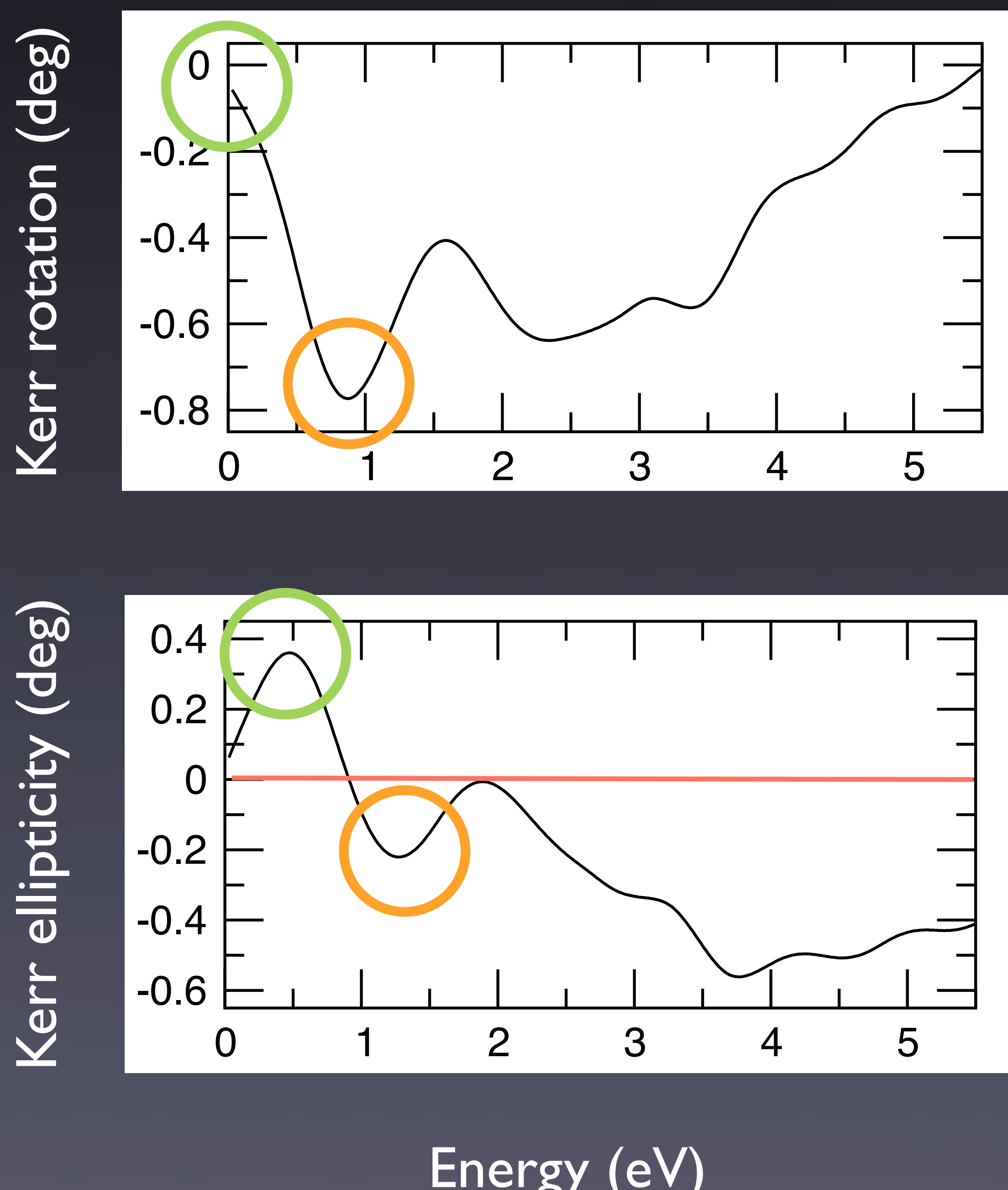


Kucera et al., JMMM 290-291, 2005

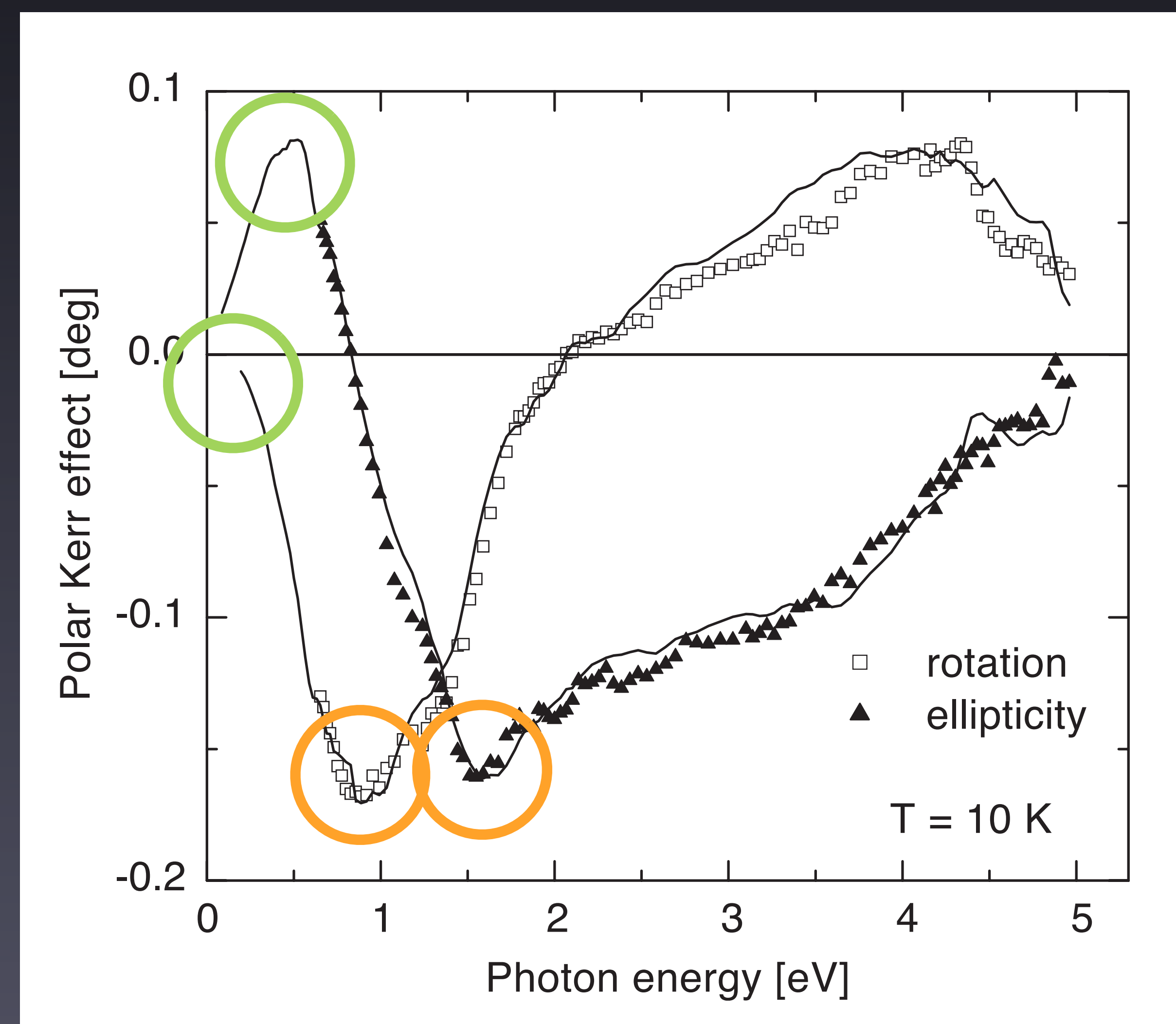
UNi_2Si_2

computed MOKE

a = 3.955 Å

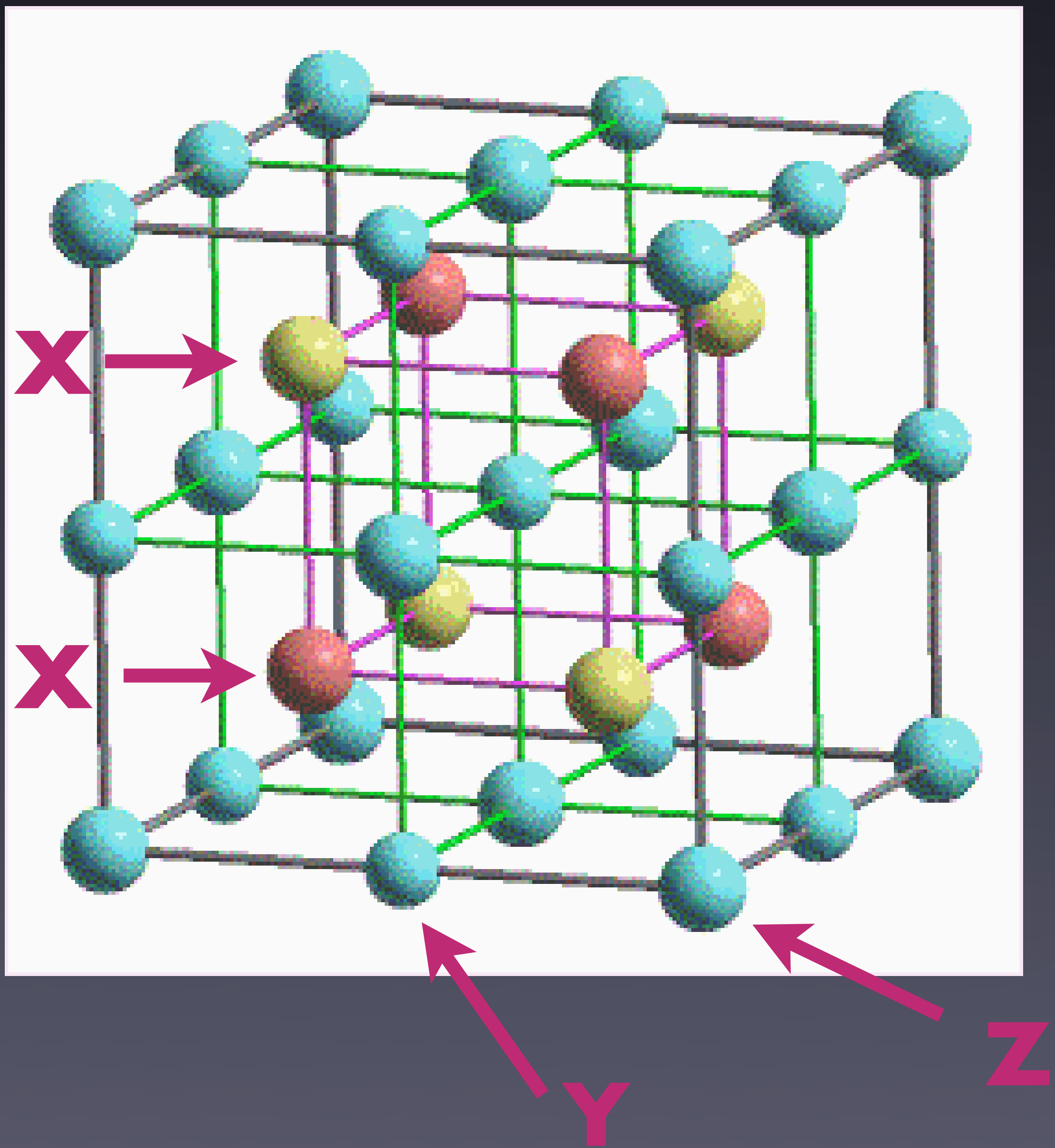


MOKE || c-axis, T = 10K, B = 4T



Kucera et al., JMMM 290-291, 2005

(half-) Heusler alloys



XYZ X_2YZ

X,Y : transition metal
Z : III / V main group element

1903 Cu_2MnAl

AuMnSn

motivation

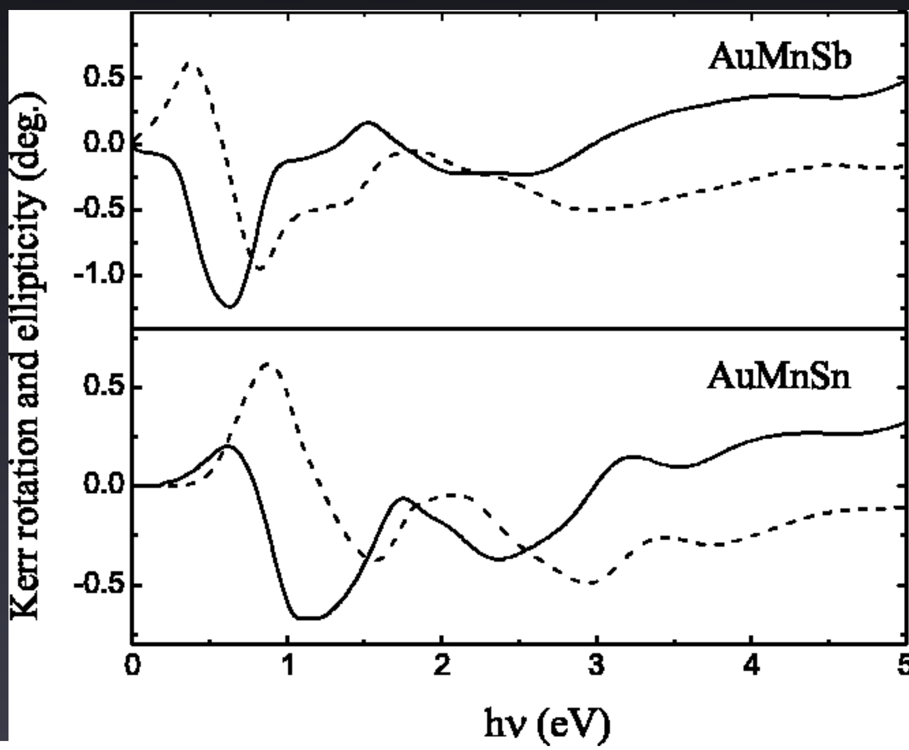
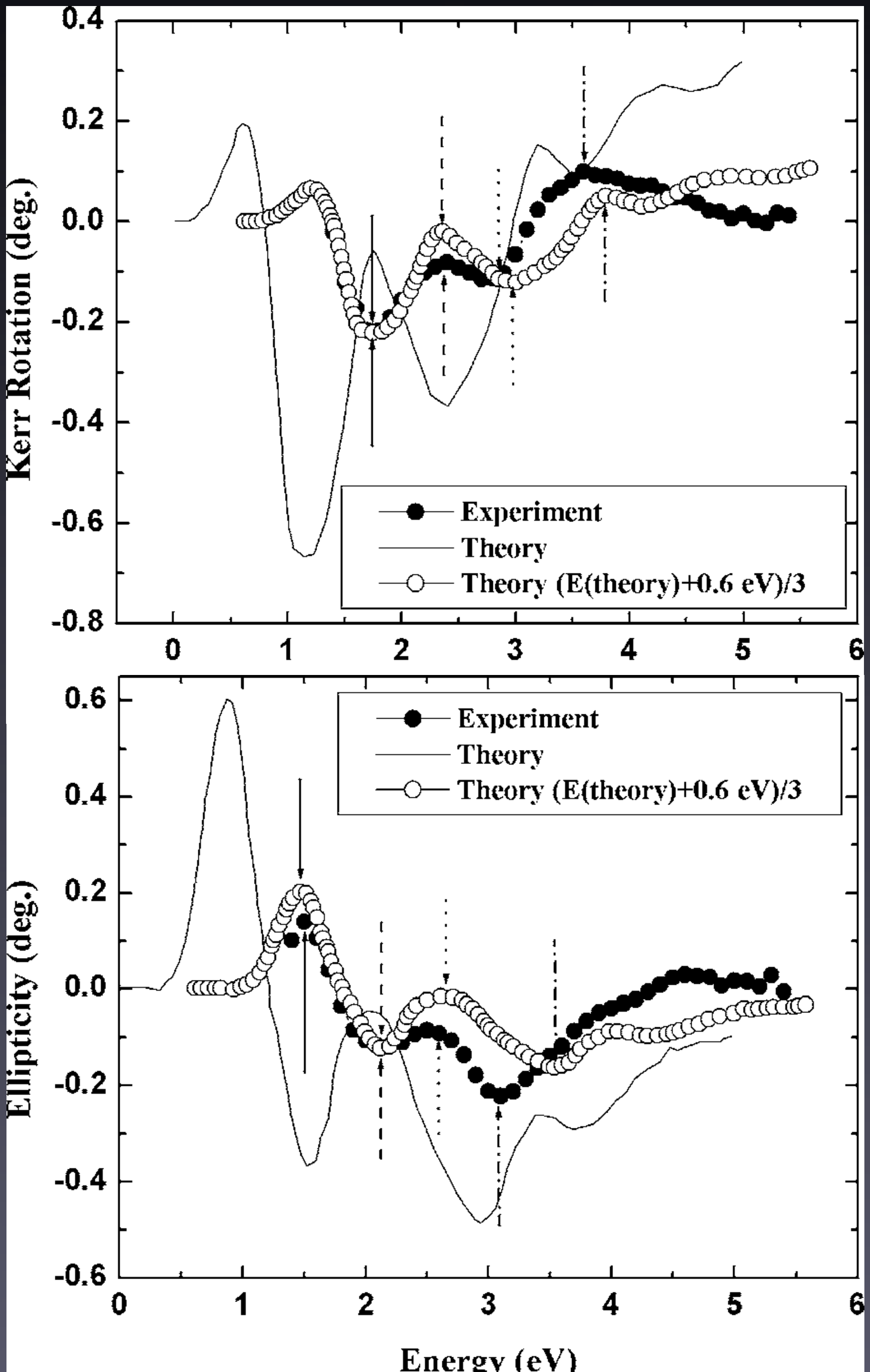


FIG. 3. Calculated (from FPLMTO) polar Kerr rotation (solid line) and ellipticity (dotted line) spectra for AuMnSb and AuMnSn.

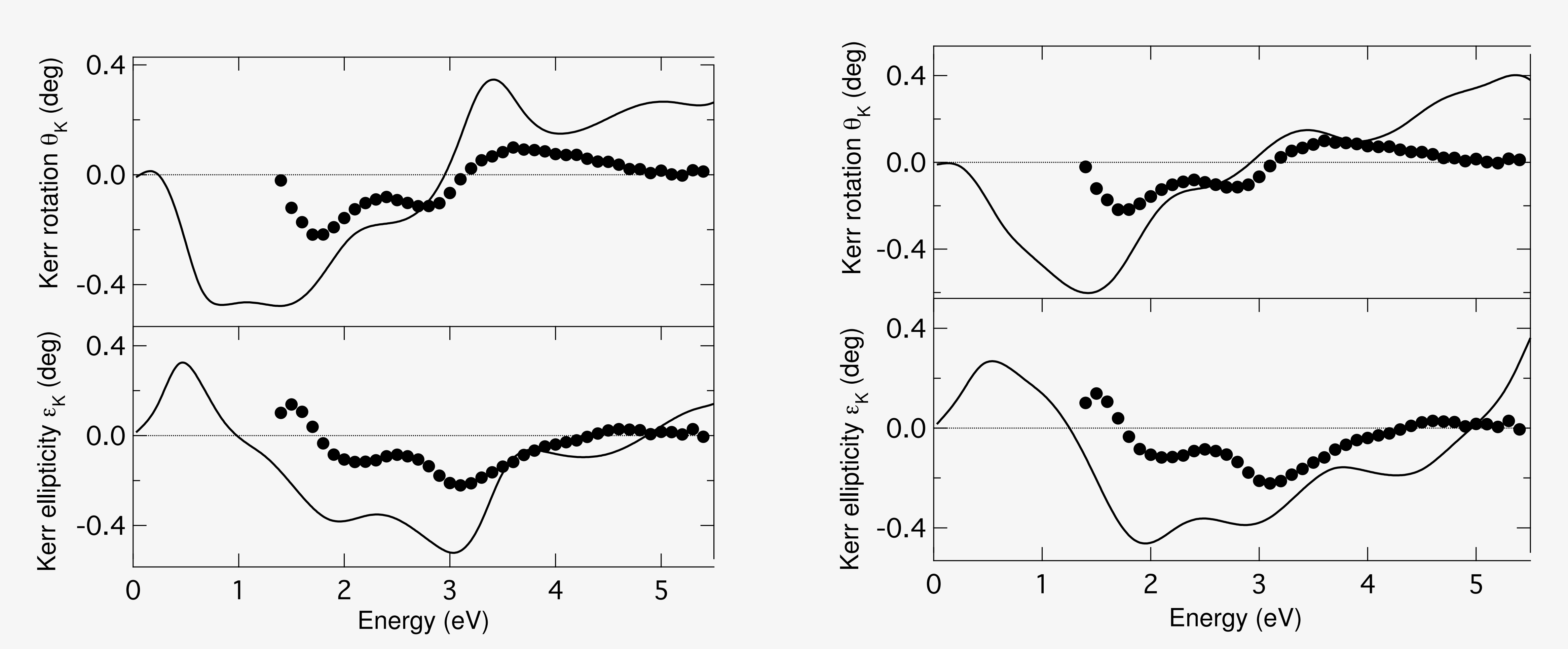
Offernes et al., APS 82, 2003



Lee et al., APS 88, 2006

AuMnSn

computed MOKE



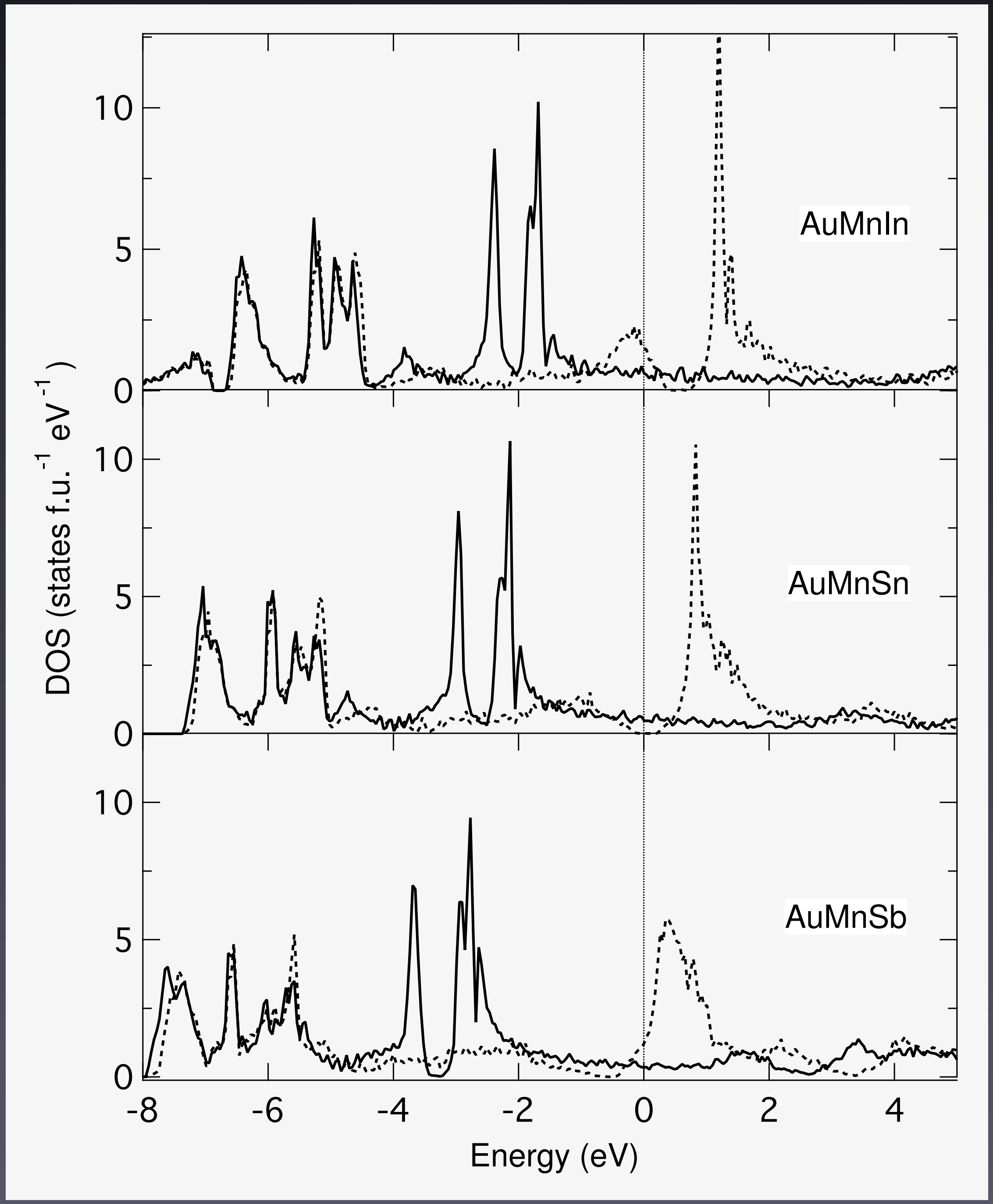
$$m_{tot}^{Mn} = 4.01\mu_B$$

$$m_{tot}^{Mn} = 3.65\mu_B$$

artificially reduced magnetic moment

AuMnX

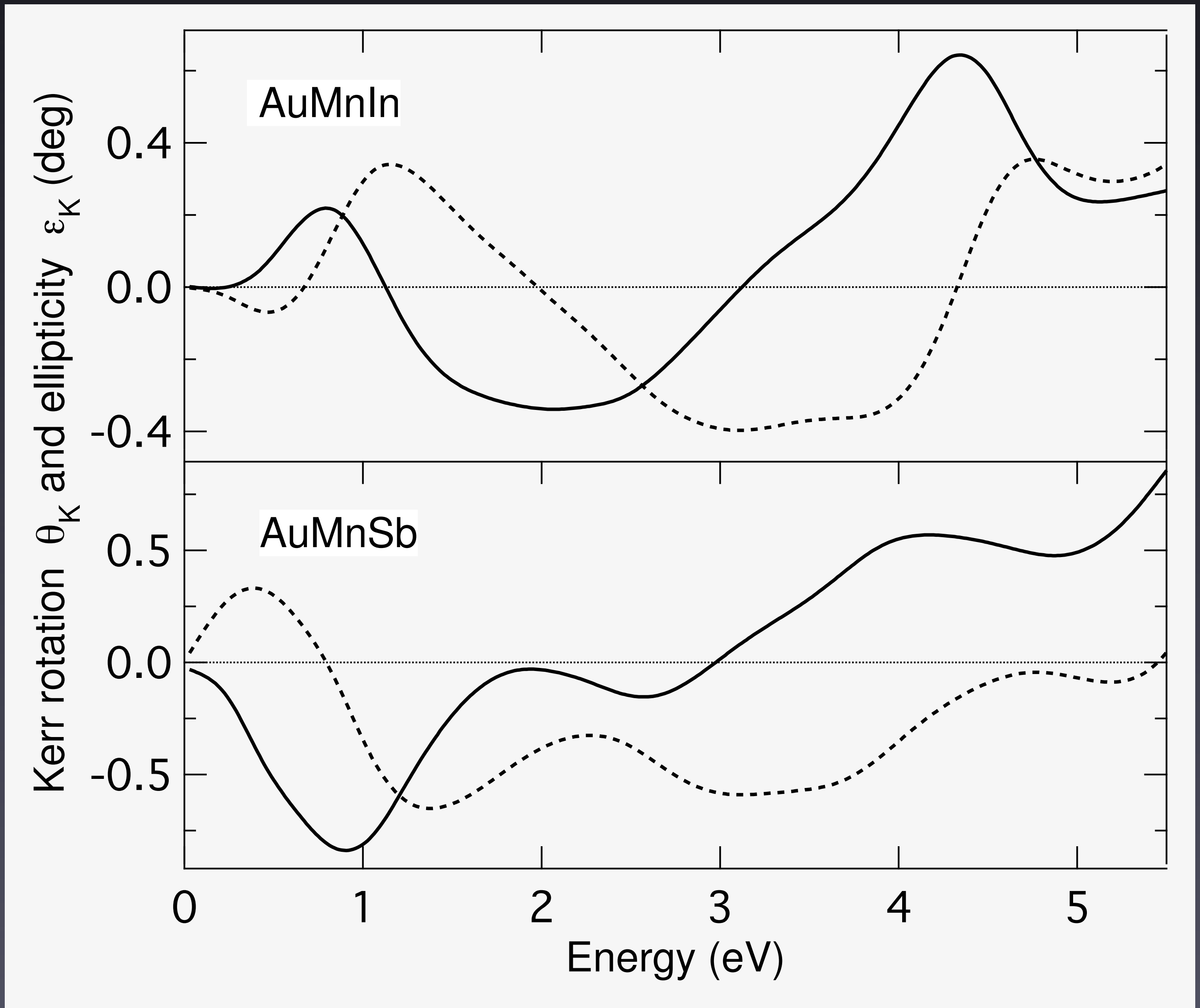
(X = In, Sn, Sb)

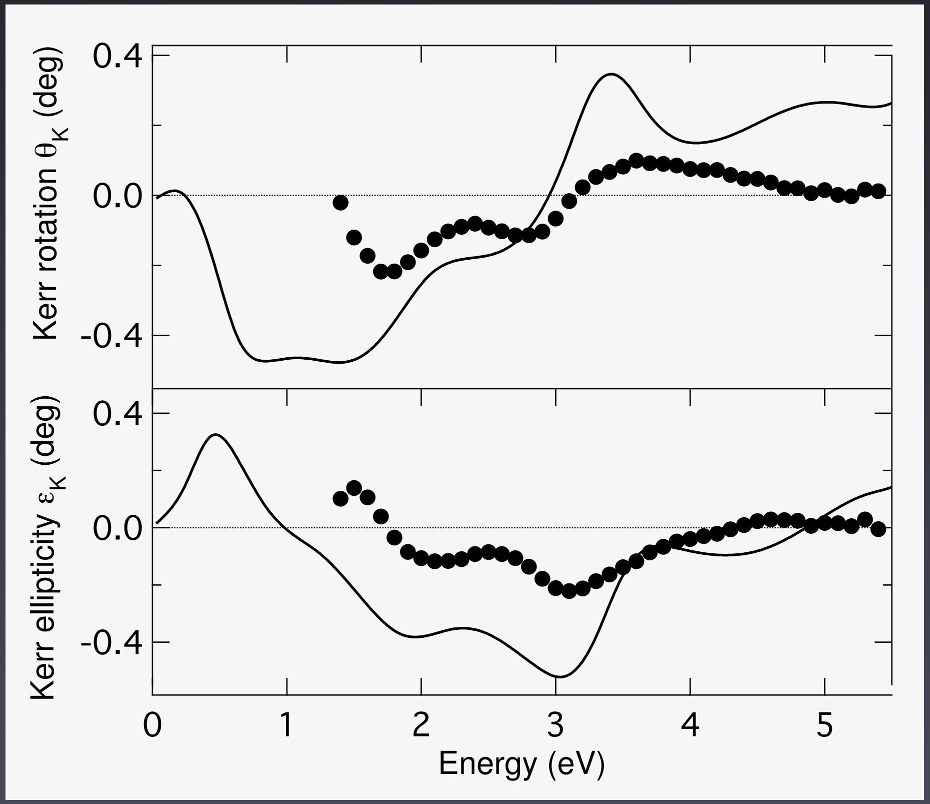


	In	Sn	Sb
Exp. a (Å)	-	6.323	6.379
Exp. m_{tot}^{Mn} (μ_B)	-	3.8±0.1	4.2±0.1
Comp. a (Å)	6.191	6.197	6.297
Comp. m_{tot}^{Mn} (μ_B)	3.79	4.01	4.24

AuMnX

(X = In, Sb)





AuMnSn

solid line: rotation
dashed line: ellipticity

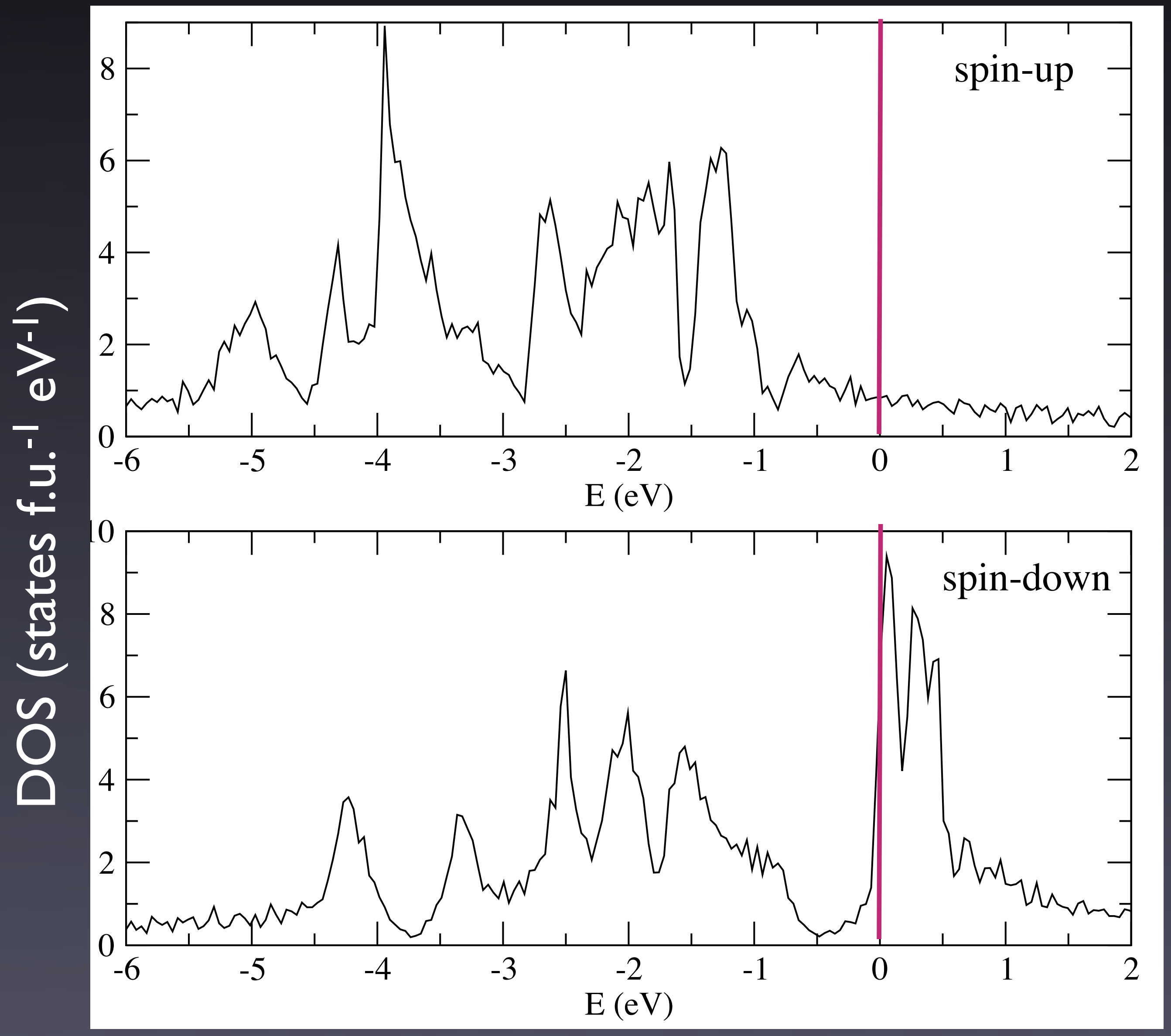
Co_2FeSi

- half metallic ferromagnet
- measured magnetic moment of $6\,\mu_B$ and Curie temperature of $1100\ \mathrm{K}$
- not reproducible by LSDA (+ GGA + ...)
- reproduced magnetic moment with LDA+U with $U_{eff,Co} = 4.8\,eV$ and $U_{eff,Fe} = 4.5\,eV$

Wurmehl et al., PRB 72, 2005
Kandpal et al., PRB 73, 2006

Co_2FeSi

experimental lattice constant

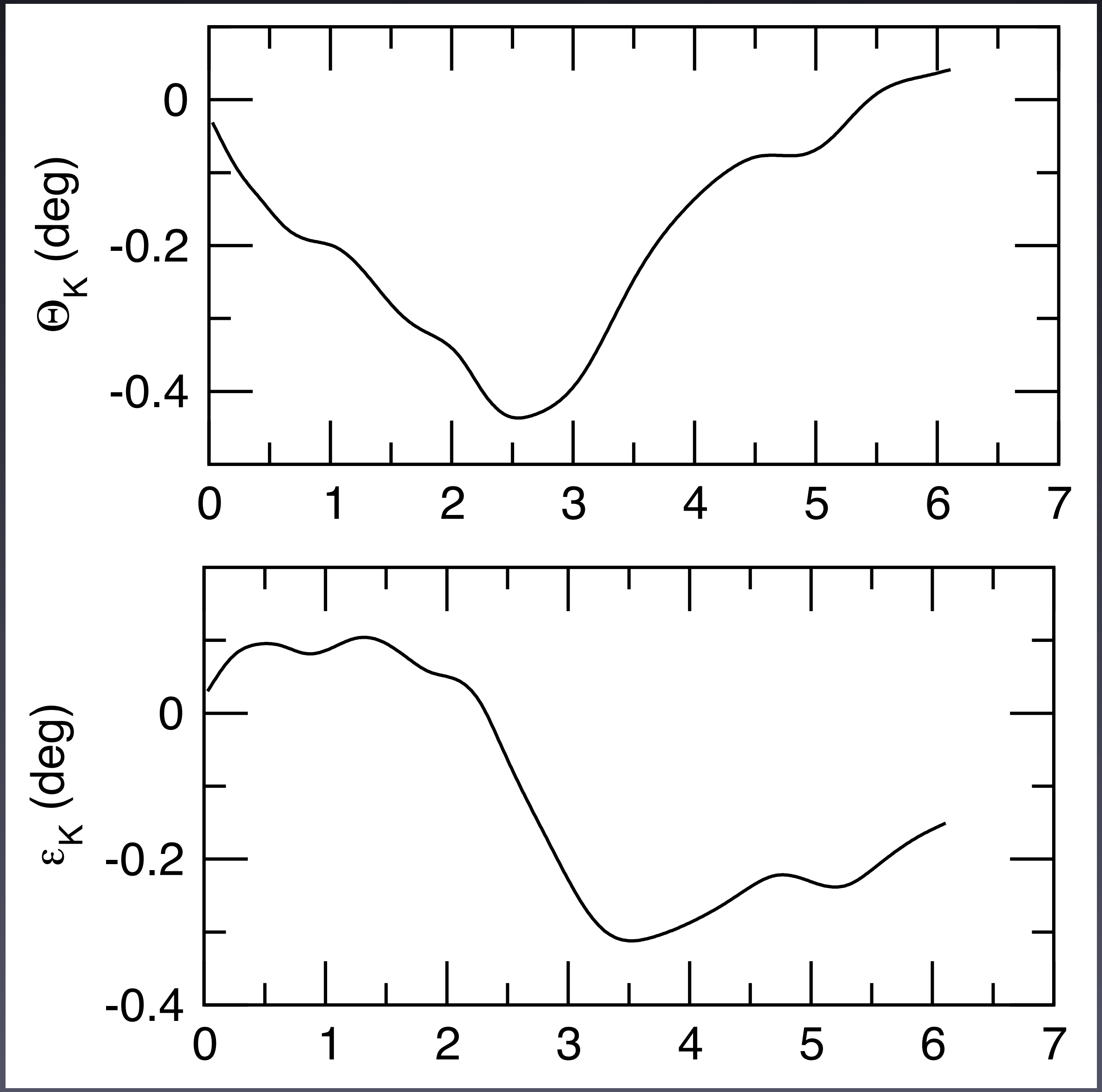


$$m_{tot}/f.u. = 5.09\,\mu_B$$

so far no experimental evidence for half-metallicity

Co_2FeSi

MOKE (exp. lattice constant)



Energy (eV)

Summary

- ASW and MOKE scheme
- Computed DOS and MOKE for UNi_2Si_2, AuMnX and Co_2FeSi

Outline

- UNi_2Si_2: AFM + external magnetic field
- band structure and Fermi surface
- using LSDA + GGA + U
- using the optical conductivity to compute other quantities, like Hall resistivity, dynamical susceptibility, ...

Thank you for your attention!

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