

Dynamika sieci w związkach aktynowców typu PuCoGa₅

P. Piekarz

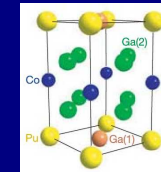
K. Parlinski, P.T. Jochym, A.M. Oleś
IFJ PAN Kraków

S. Raymond, J. P. Sanchez
DRFMC CEA Grenoble

M. Krisch, J. Serrano
ESRF Grenoble

J. Rebizant, B. Janousova, G.H. Lander
ITU Karlsruhe

N. Metoki, K. Kaneko
JAEA Tokai

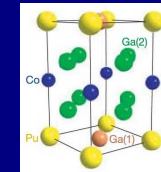


Nadprzewodnictwo ciężkich fermionów

	T_c [K]	γ [mJ/mol K ²] $\sim m^*$	f
U Be ₁₃	0.86	~1000	4f ¹
Ce Cu ₂ Si ₂	0.7		
Ce CoIn ₅	2.3	~250	4f ¹
Pu CoGa ₅	18.5	~77	5f ⁶
Np CoGa ₅	T _N =47 K	~64	5f ⁴
U CoGa ₅	paramagnetyk	~10	5f ³



PuCoGa₅ Nature 420, 297 (2002)



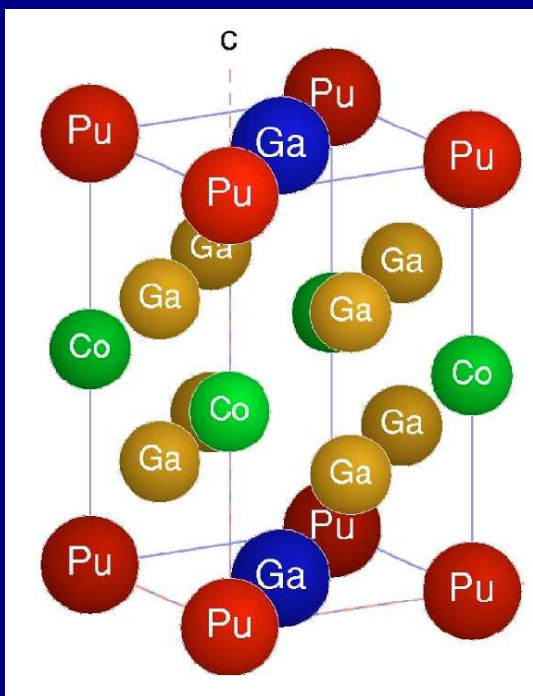
Plutonium-based superconductivity with a transition temperature above 18 K

J. L. Sarrao*, L. A. Morales*, J. D. Thompson*, B. L. Scott*,
G. R. Stewart*†, F. Wastin‡, J. Rebizant‡, P. Boulet‡, E. Colineau‡
& G. H. Lander*‡

* Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

† Department of Physics, University of Florida, Gainesville, Florida 32611, USA

‡ European Commission, JRC, Institute for Transuranium Elements, Postfach
2340, 76125 Karlsruhe, Germany

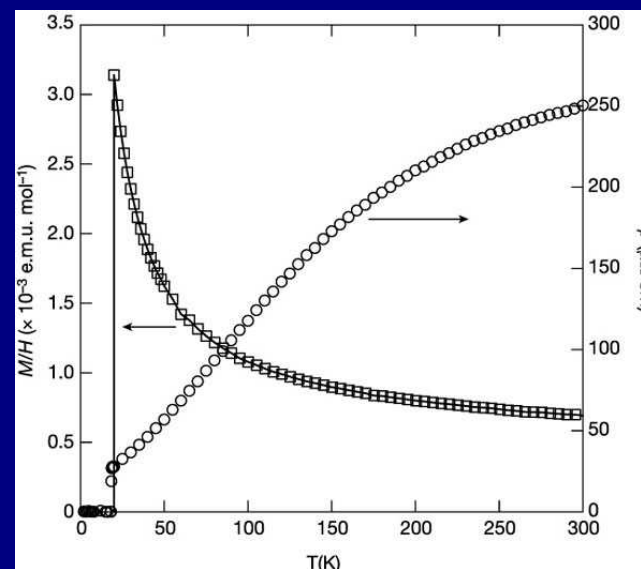
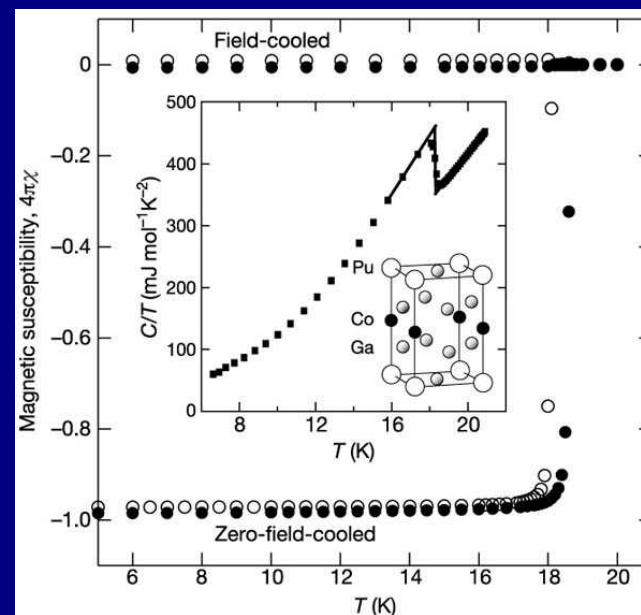


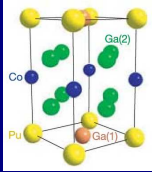
P4/mmm

$a = 4.232$

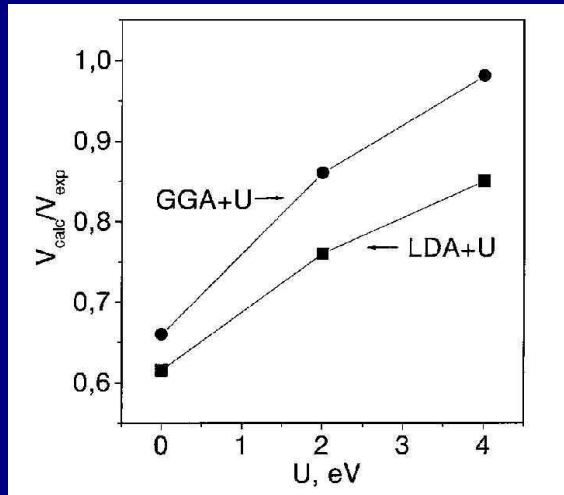
$c = 6.786$

$z = 0.312$

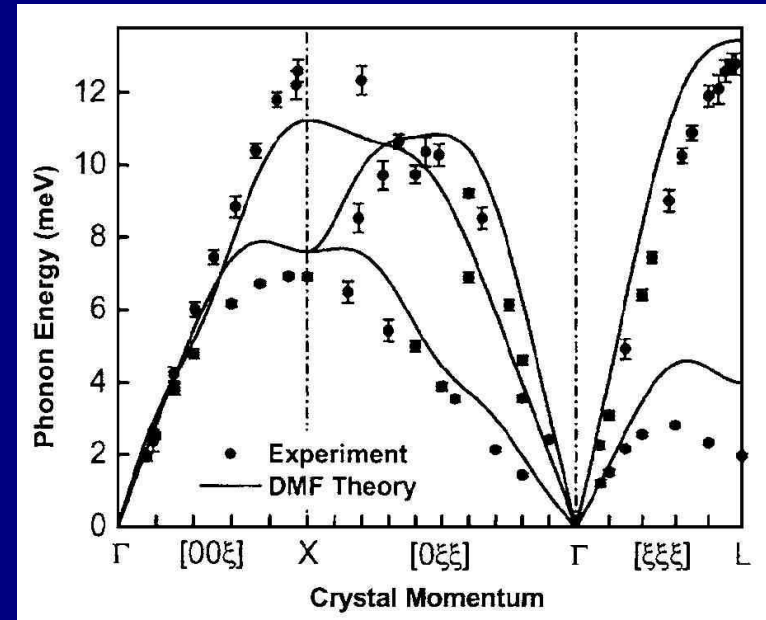




Pu - δ

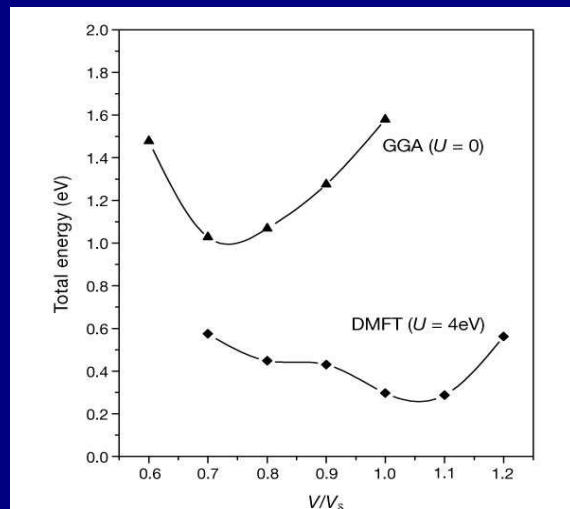


S.Y. Savrasov and G. Kotliar
PRL 84, 3670 (2000)

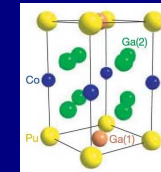


X. Dai, S.Y. Savrasov, G. Kotliar, A. Migliori, H. Ledbetter
and E. Abrahams, Science 300, 953 (2003)

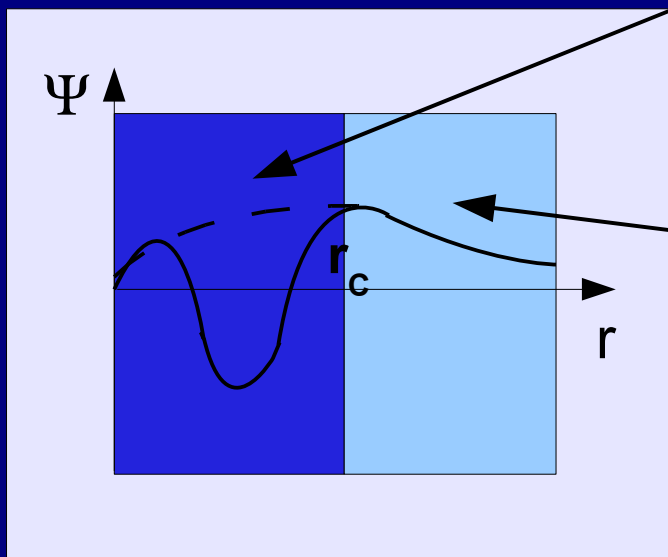
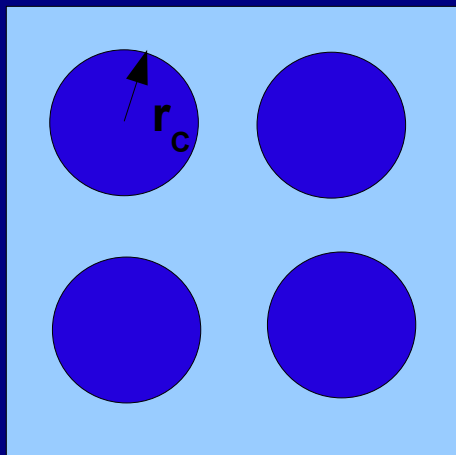
J. Wong, M. Krisch, D.L. Farber, F. Occelli, A.J. Schwartz,
T.C. Chiang, M. Wall, C. Boro, R. Xu, Science 301, 1078 (2003)



S.Y. Savrasov, G. Kotliar, and E. Abrahams,
Nature 410, 793 (2001)



Projector augmented - wave (PAW) method P.E. Blochl, PRB 50, 17953 (1994), G. Kresse, D. Joubert - VASP



DFT - GGA - PAW

$$H = T[n] + V^H[n] + V^{xc}[n] + V^{ion}[n]$$

$$H|\Psi^p\rangle = E|\Psi^p\rangle \quad (\text{K-S})$$

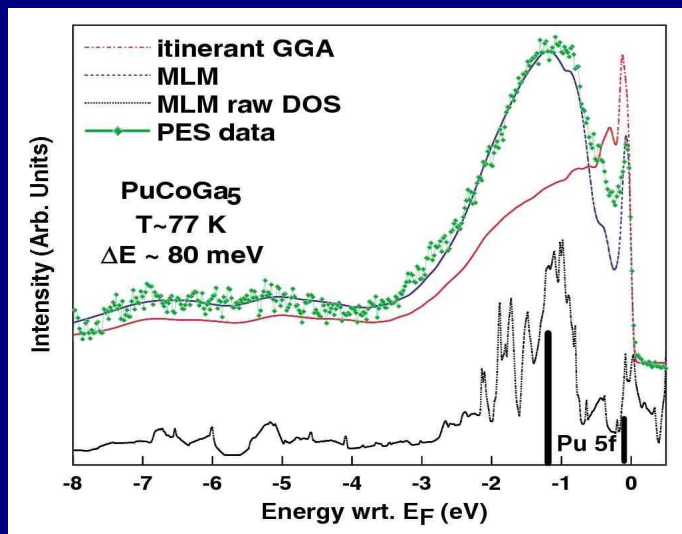
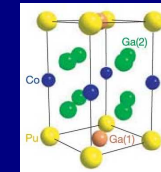
$$\begin{aligned} r < r_c \quad |\Psi\rangle &= \sum_i c_i |\phi_i\rangle \\ |\Psi^p\rangle &= \sum_i c_i |\phi_i^p\rangle \\ c_i &= \langle p_i | \Psi^p \rangle \end{aligned}$$

$$r > r_c \quad |\Psi\rangle = |\Psi^p\rangle = \sum_G c_G e^{iGr}$$

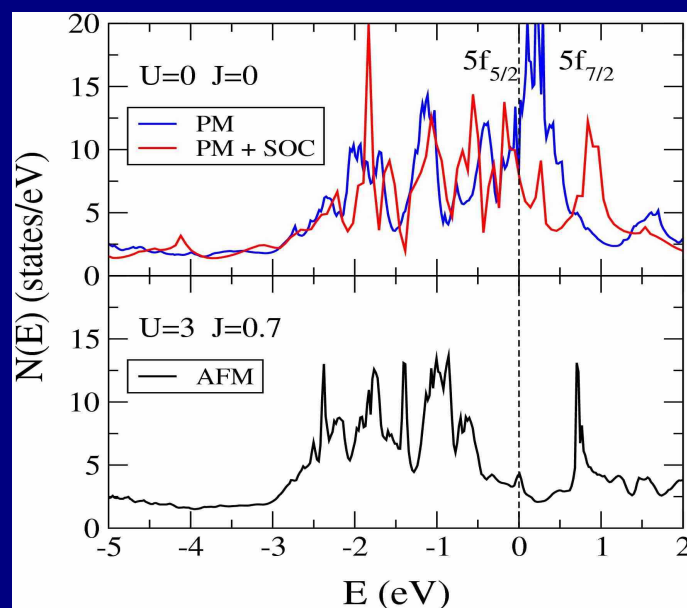
$$\frac{\hbar^2}{2m} |G|^2 < E_{\text{cutoff}} = 520 \text{ eV}$$

$$|\Psi\rangle = |\Psi^p\rangle + \sum_i (|\phi_i\rangle - |\phi_i^p\rangle) \langle p_i | \Psi^p \rangle$$

Struktura elektronowa – silne korelacje w stanach Pu 5f

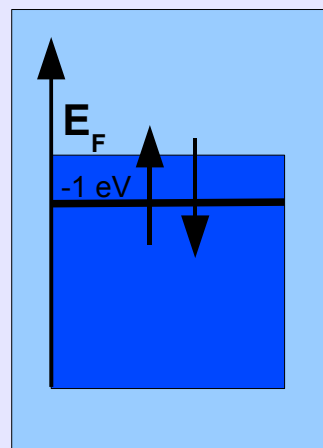


J.J. Joyce *et al.* PRL 91, 176401 (2003)



GGA+U

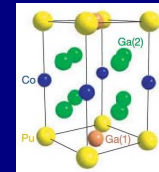
$$E_{\text{tot}} = E_{\text{GGA}} + E_U - E_{\text{DC}} = \min$$



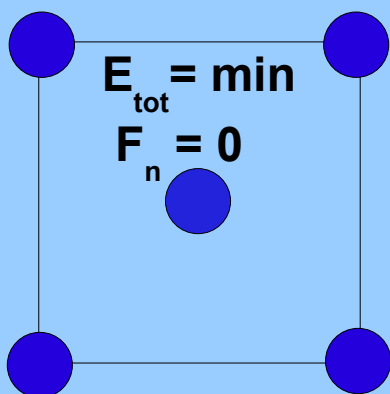
$$E_U = U \sum_{i\alpha\beta\sigma} n_{i\alpha\sigma} n_{i\beta-\sigma} + (U - J) \sum_{i\alpha<\beta\sigma} n_{i\alpha\sigma} n_{i\beta\sigma}$$

$$n_{\alpha\sigma} = |\langle m_{\alpha} | \Psi_{\sigma} \rangle|^2$$

	U=J=0 NM	U=3, J=0.7 eV FM	AF	exp
a	4.197	4.230	4.236	4.232
c/a	1.595	1.641	1.630	1.603
z	0.304	0.312	0.311	0.312



Program PHONON – K. Parlinski (direct method)



$$F = - dE_{\text{tot}}/du \quad (\text{siły H-F})$$

$$F_n = - \sum_m \Phi_{nm} u_m$$

Φ_{nm} - stałe siłowe

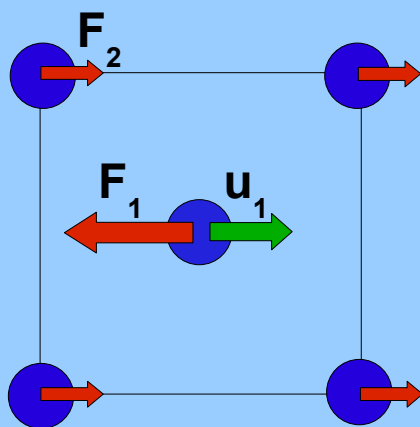
Macierz dynamiczna $D(k)$

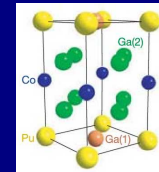
$$D(k) = 1/m \sum_m \Phi_{0m} \exp[-ik(r_m - r_0)]$$

$$D(k)e(k) = \omega^2(k)e(k)$$

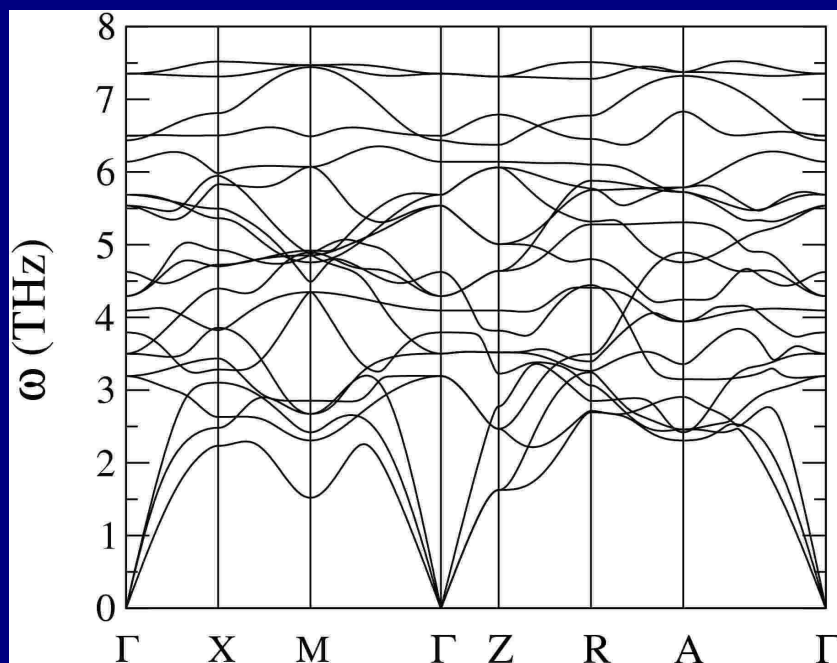
$\omega(k)$ - relacje dyspersji

$e(k)$ - wektory polaryzacji

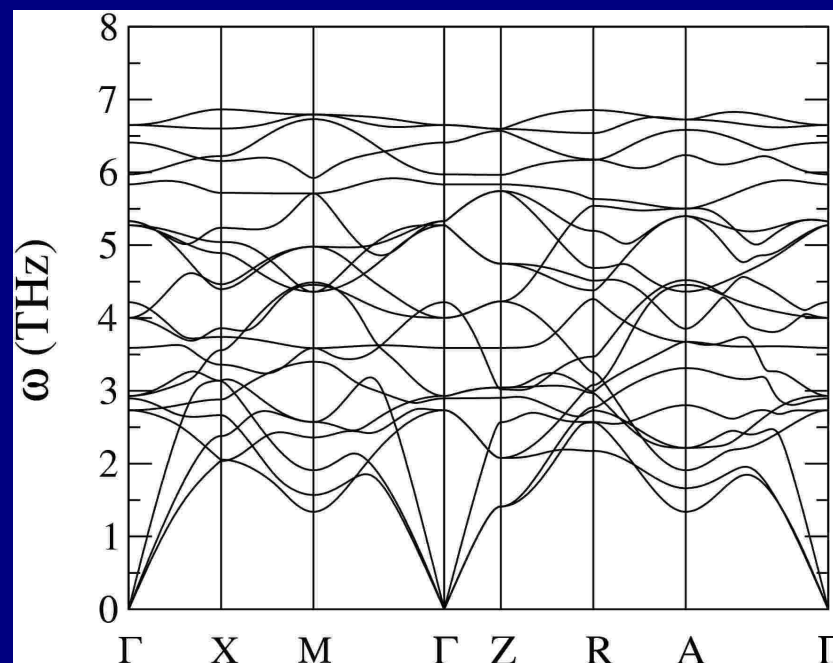




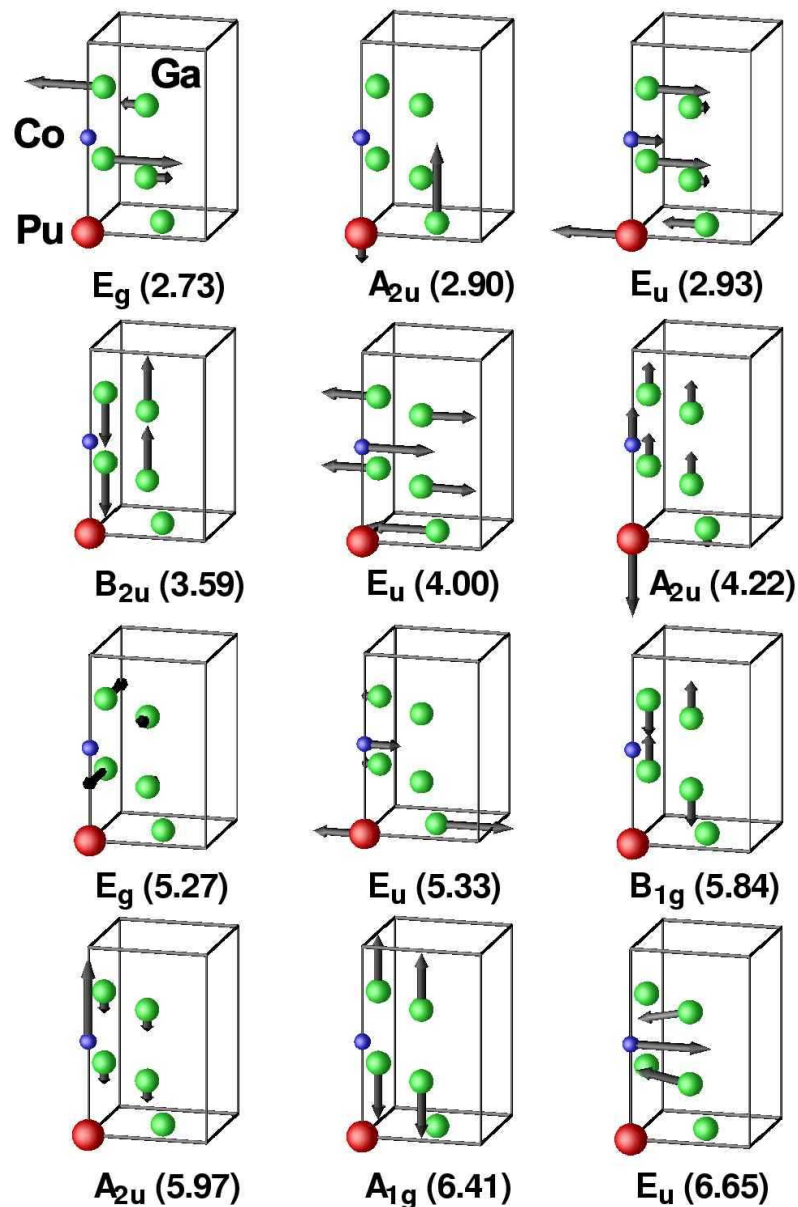
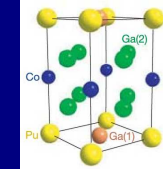
$U = 0 \quad J = 0$



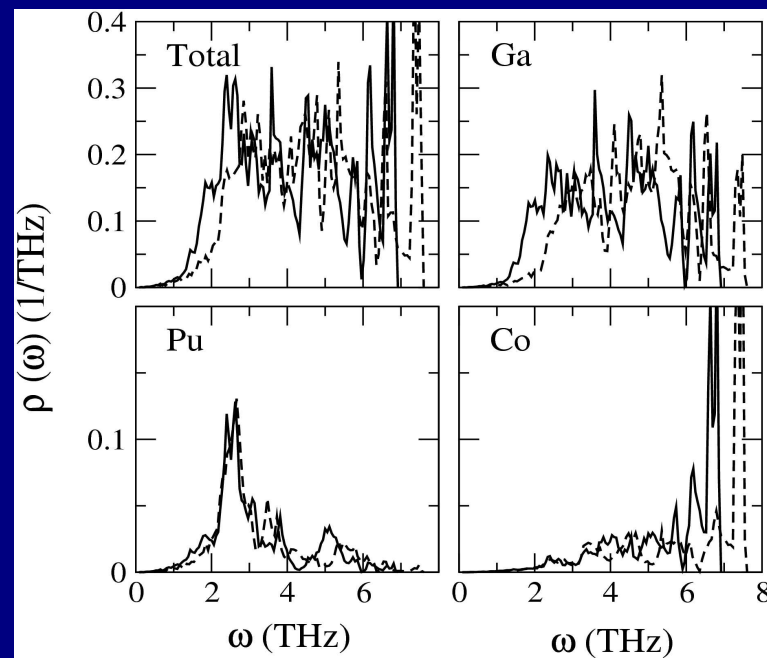
$U = 3 \text{ eV} \quad J = 0.7 \text{ eV}$

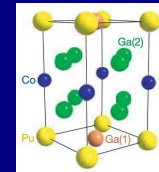


P. Piekarz, P.T. Jochym, K. Parlinski, A.M. Oleś, J.P. Sanchez, J. Rebizant, PRB 72, 014521 (2005)



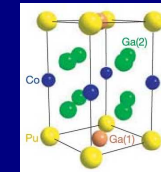
Γ	$U = 3 \text{ eV}$	$U = 0$	$\delta(U)$	active
E_g	2.733	3.192	17	R
A_{2u}	2.896	3.815	32	I
E_u	2.929	3.691	26	I
B_{2u}	3.589	4.097	14	—
E_u	4.002	4.297	7	I
A_{2u}	4.216	4.623	10	I
E_g	5.273	5.688	8	R
E_u	5.330	5.585	5	I
B_{1g}	5.835	6.151	5	R
A_{2u}	5.972	6.406	7	I
A_{1g}	6.409	6.619	3	R
E_u	6.650	7.365	11	I





ESRF – ILL - Grenoble





European Synchrotron Radiation Facility Grenoble

ID28 undulator beamline

Monochromator

Si(111) $E=21.747$ keV

Rozdzielczość: 1.5 meV

Próbki:

$1.3 \times 0.55 \times 0.33 \text{ mm}^3$

$0.5 \times 1 \times 0.04 \text{ mm}^3$

$0.5 \times 0.15 \times 0.02 \text{ mm}^3$

Experimental set-up

Monochromator:

Si(n,n,n), $\theta_b = 89.98^\circ$

$n=7-13$

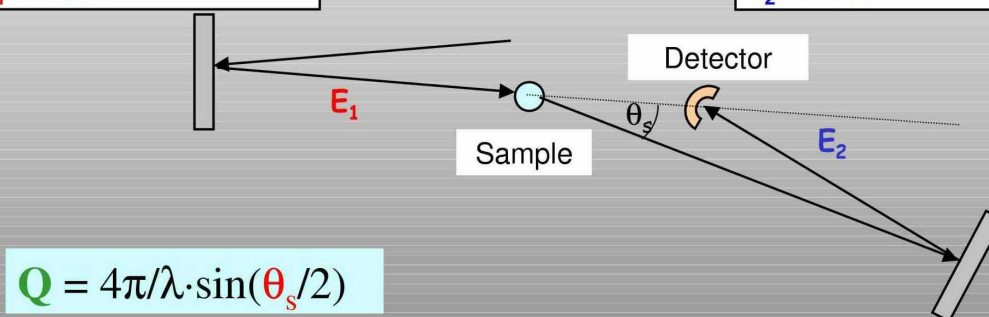
λ_1 **tunable**

Analyser:

Si(n,n,n), $\theta_b = 89.98^\circ$

$n=7-13$

λ_2 **constant**

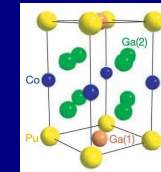


$$Q = 4\pi/\lambda \cdot \sin(\theta_s/2)$$

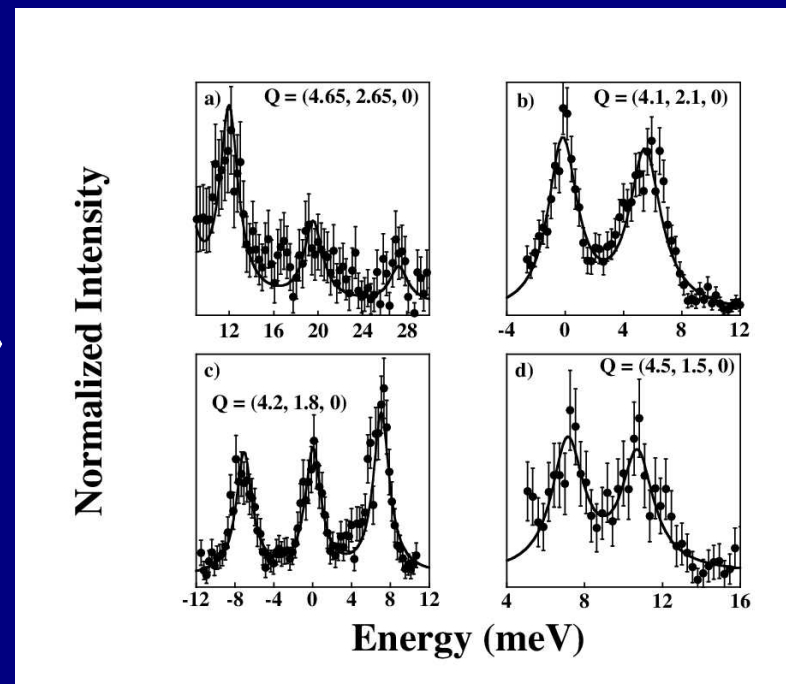
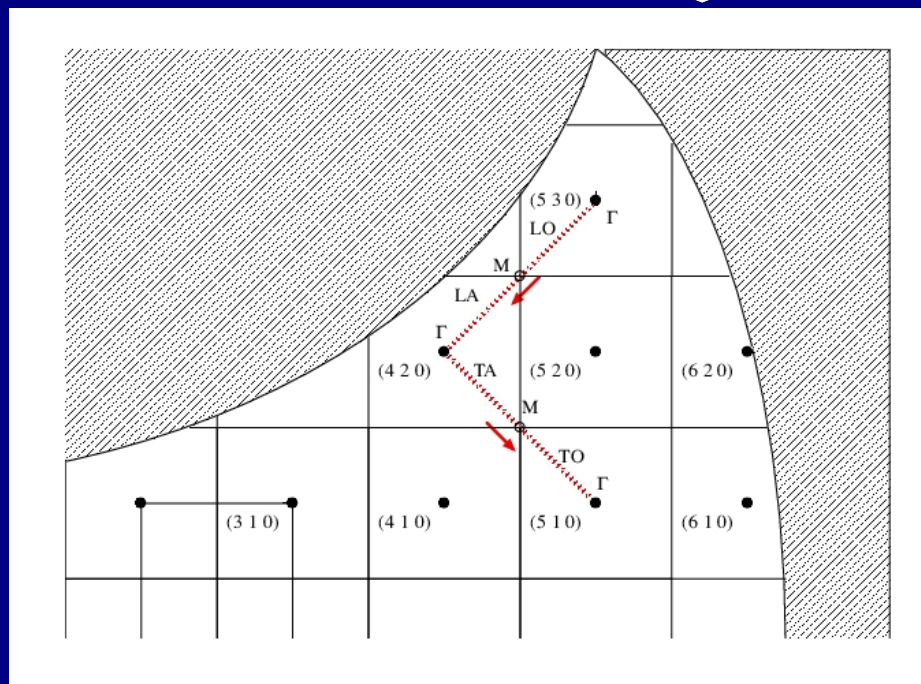
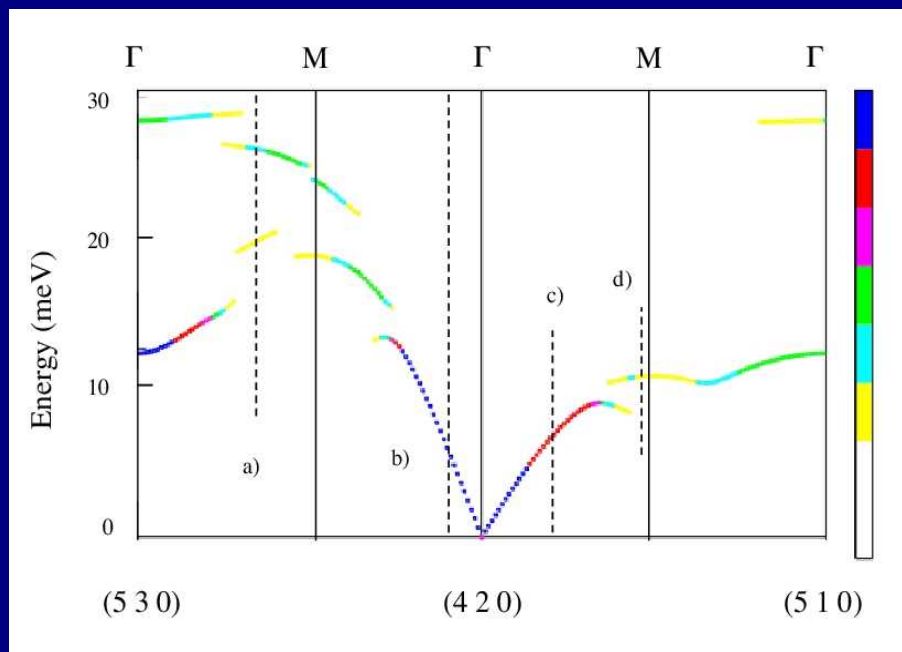
$$\lambda = 2 \cdot d(T) \sin\theta_B$$

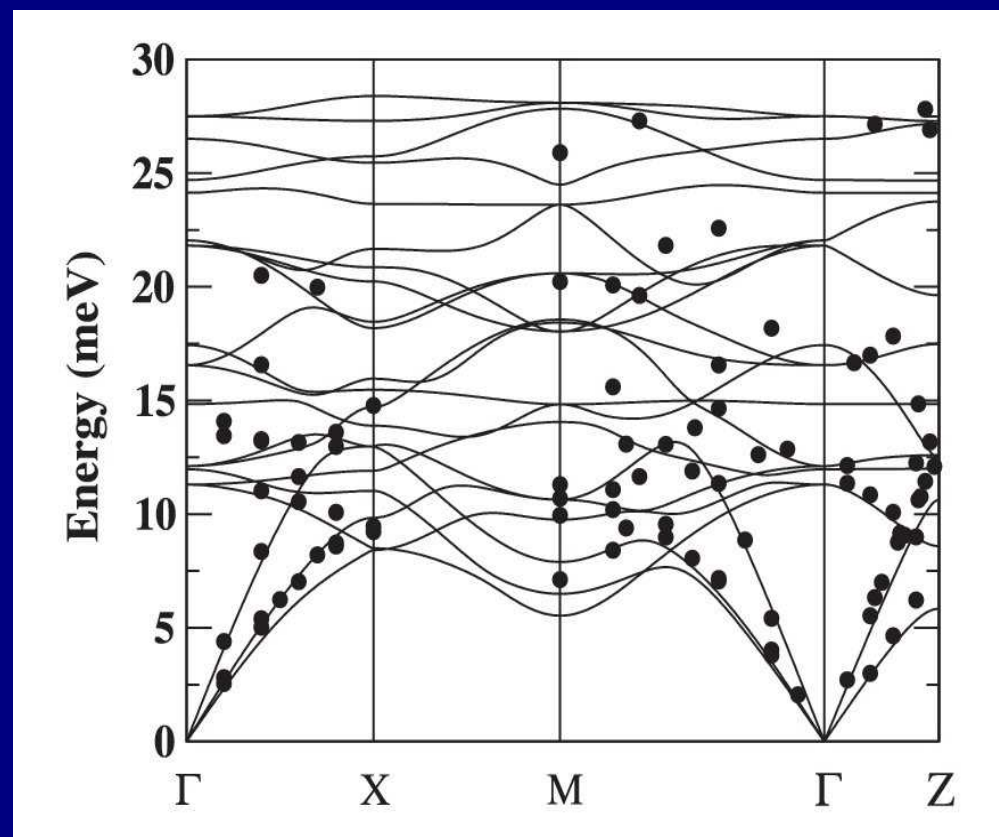
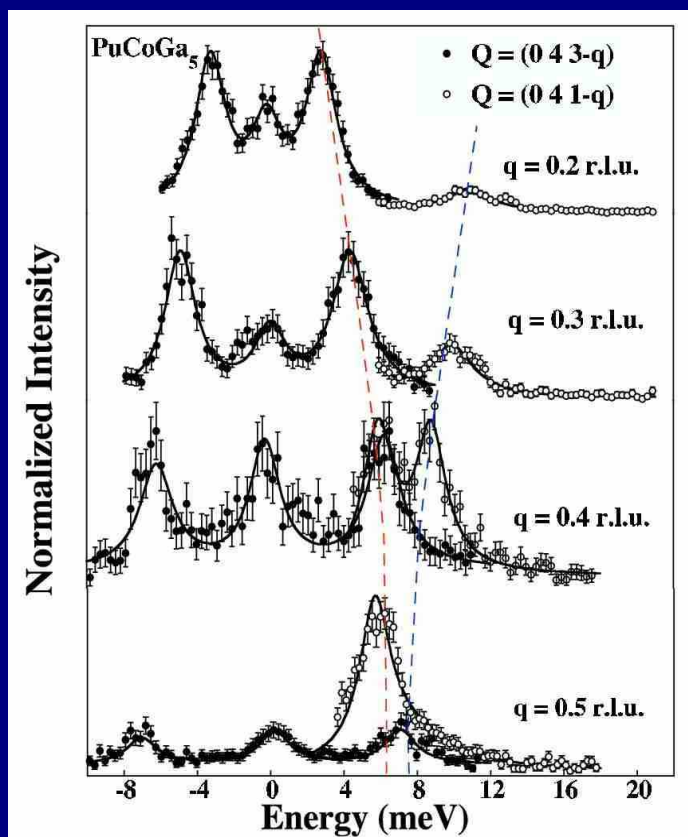
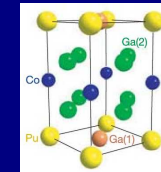
$$\Delta d/d = \Delta E/E = -\alpha(T) \cdot \Delta T \quad (\alpha = 2.58 \cdot 10^{-6} \text{ at RT})$$

Beam size: $30 \text{ (250)} \times 70 \mu\text{m}^2$ (hor. x vert.)

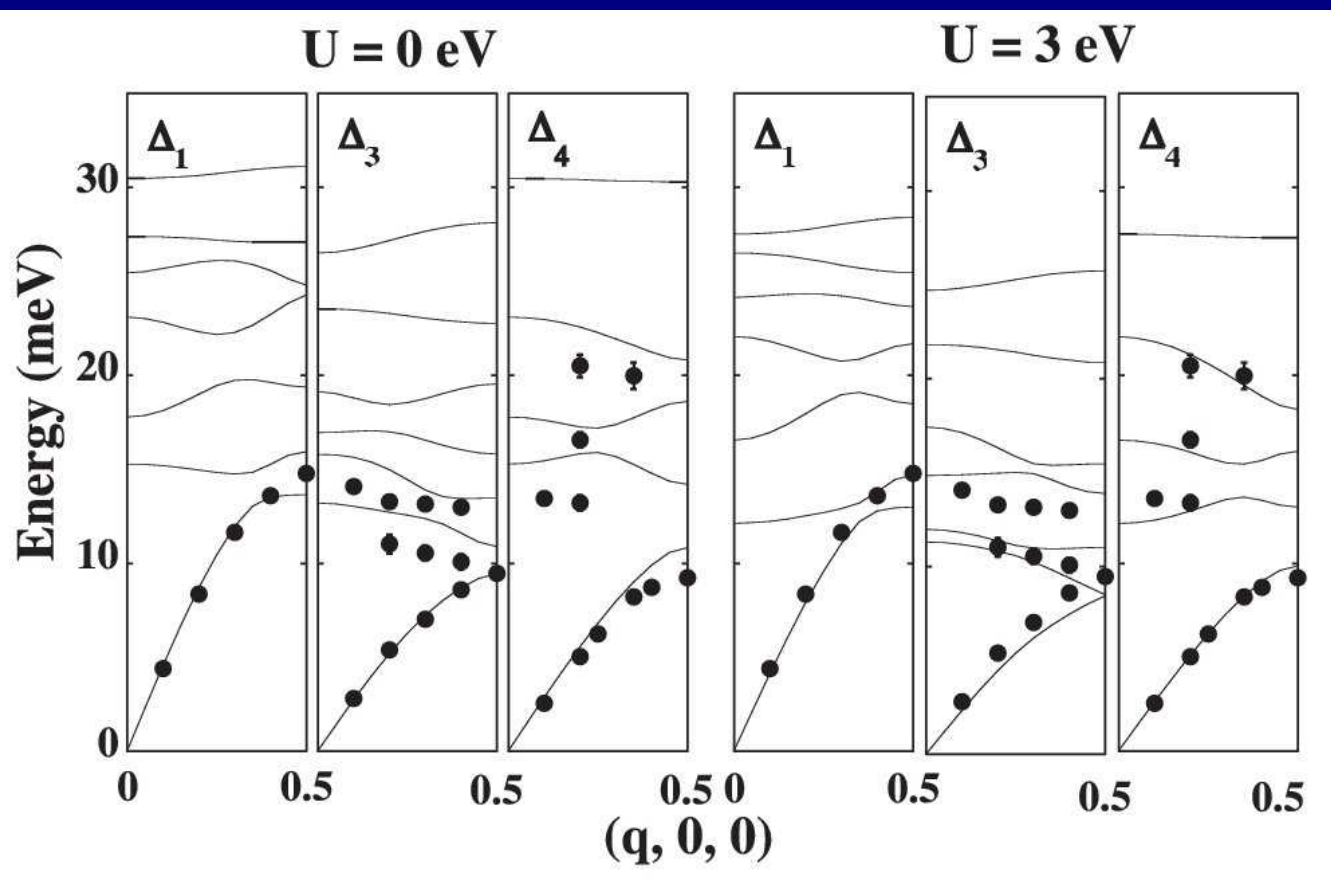
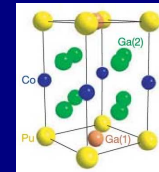


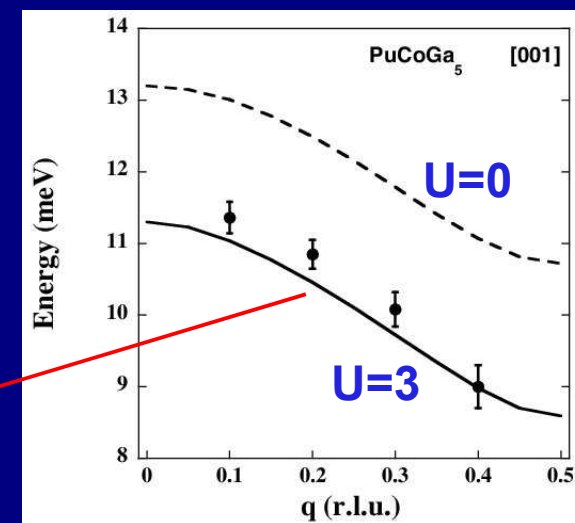
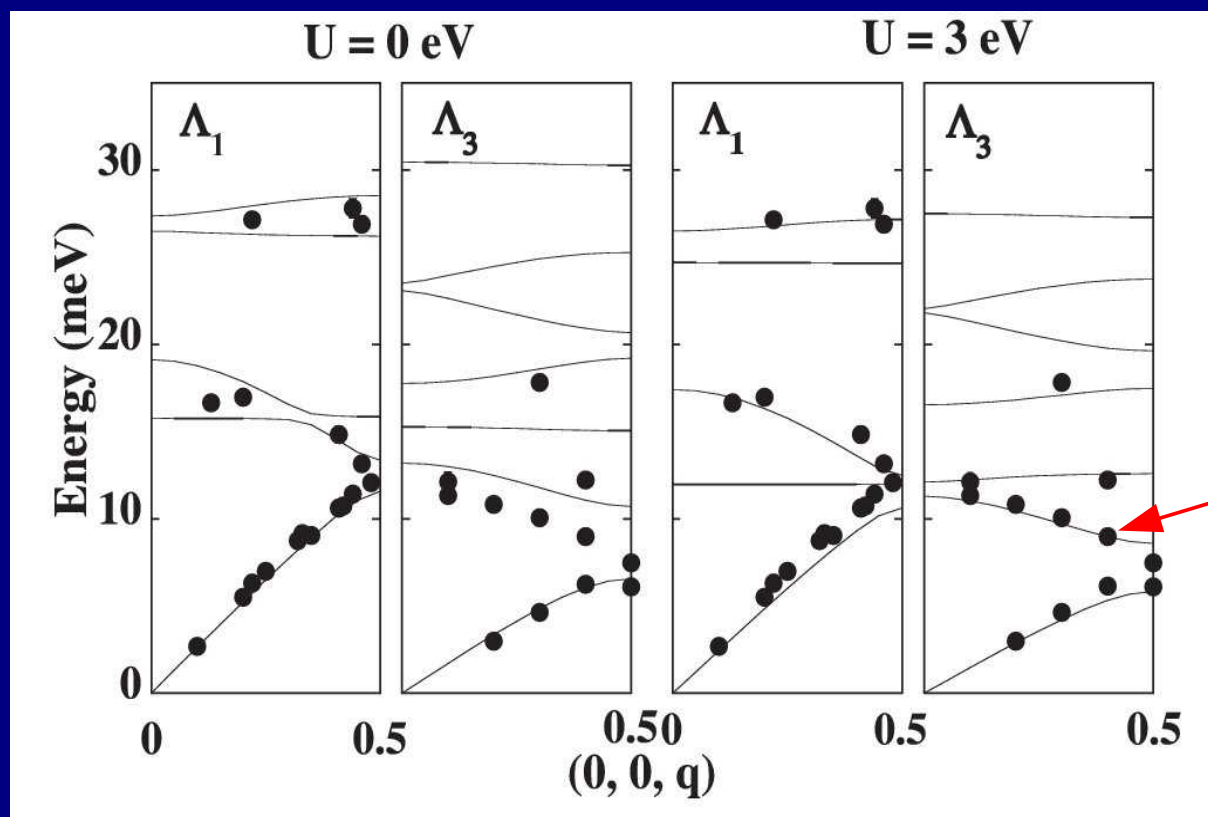
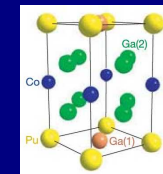
Nieleistyczne rozpraszanie promieni X

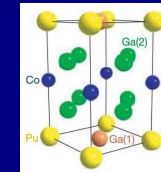




S. Raymond, P. Piekarz, J.P. Sanchez, J. Serrano, M. Krisch, B. Janousova, J. Rebizant, N. Metoki, K. Kaneko, P.T. Jochym, A.M. Oleś, and K. Parlinski, PRL 96, 237003 (2006)







Institut Laue-Langevin Grenoble

High Flux Reactor $1.5 \cdot 10^5$ neutrons/sec cm^2

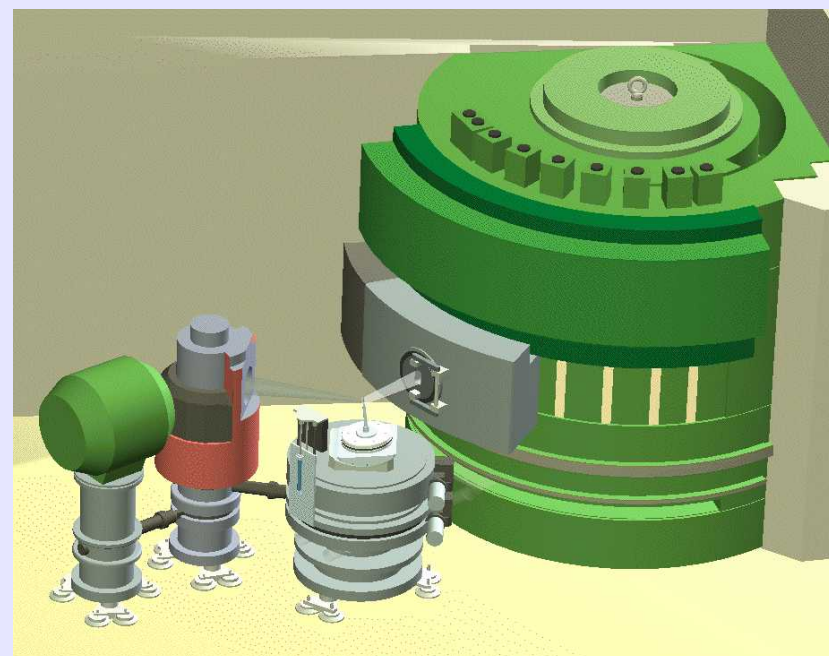
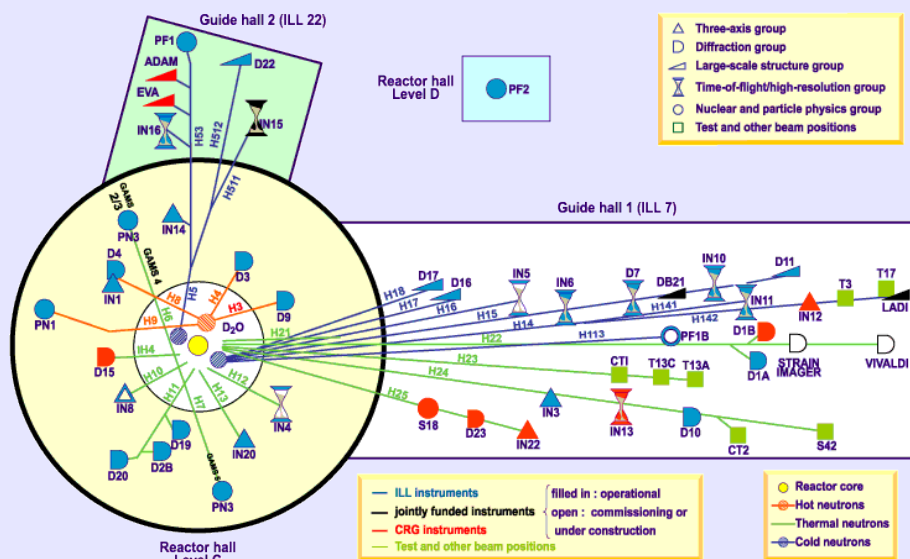
IN8 spektrometr trójosiowy

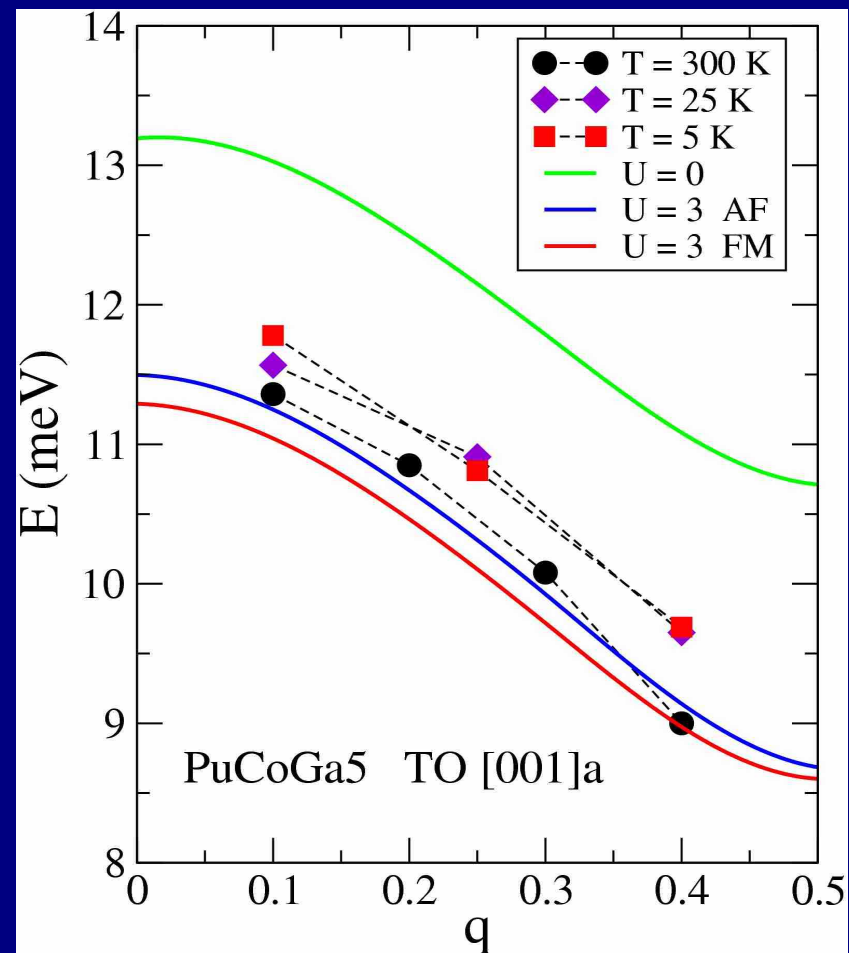
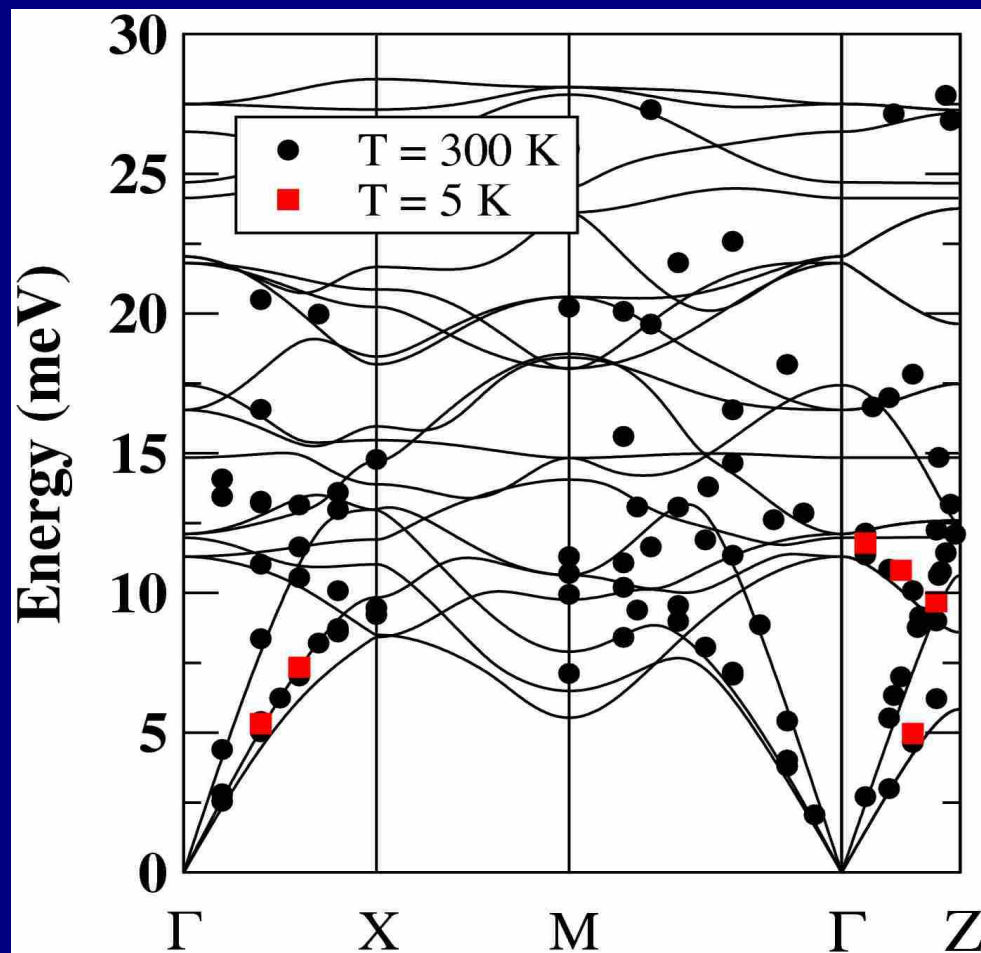
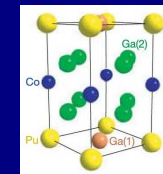
Monochromatory:

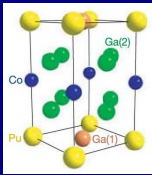
PG(002), Cu(200), Si(111)

Próbka: $4.5 \times 2.3 \times 2 \text{ mm}^3$

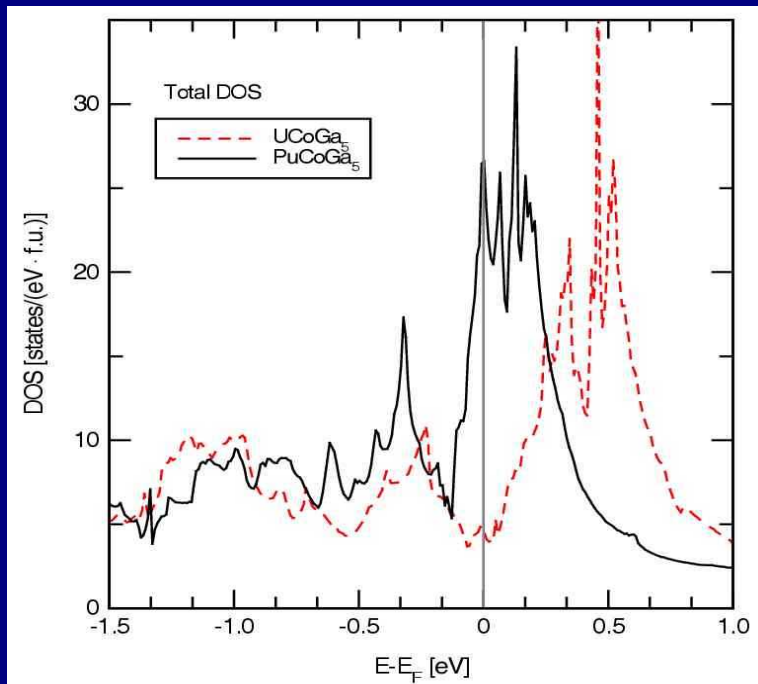
Analizator: Si (111)



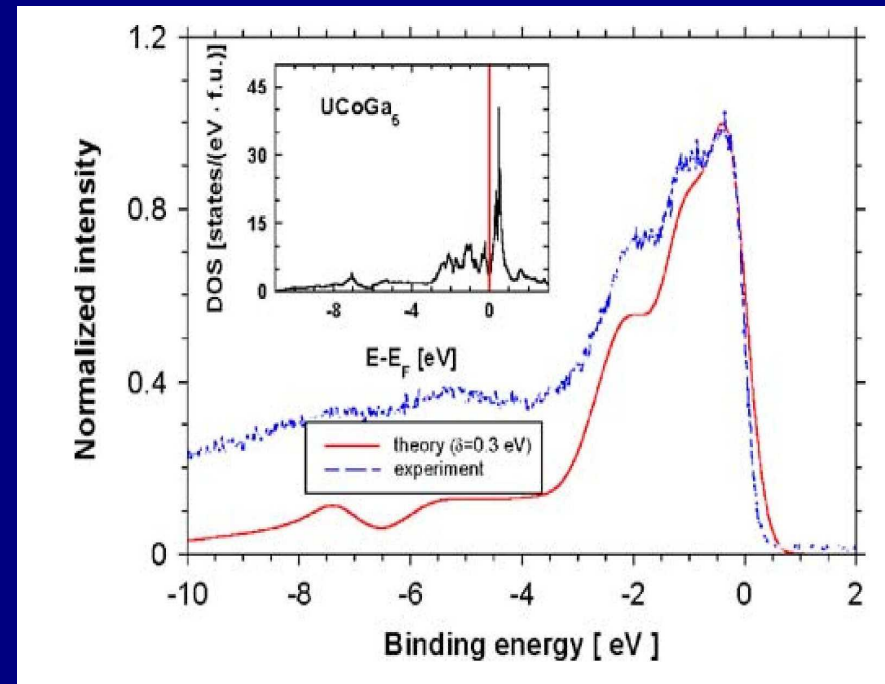




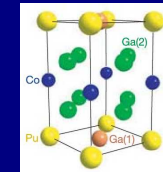
UCoGa_5



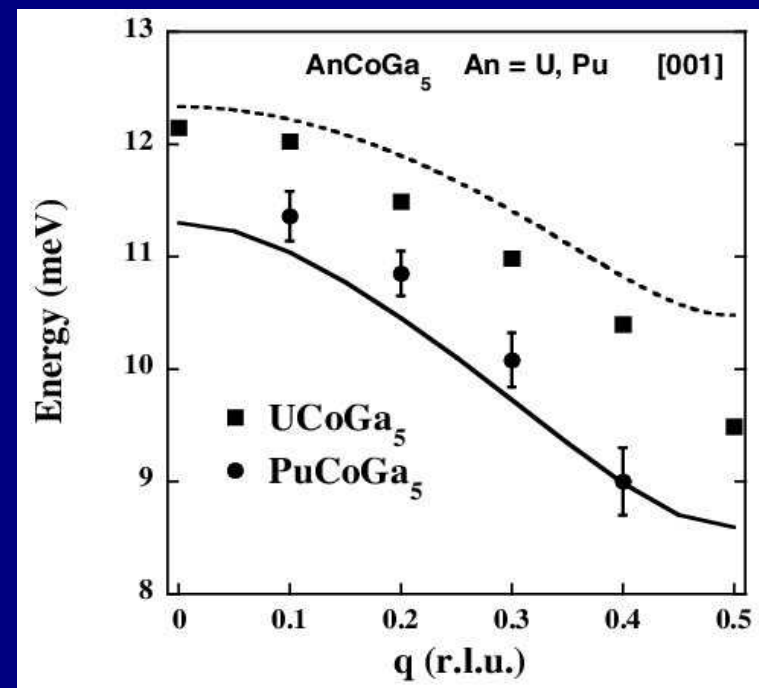
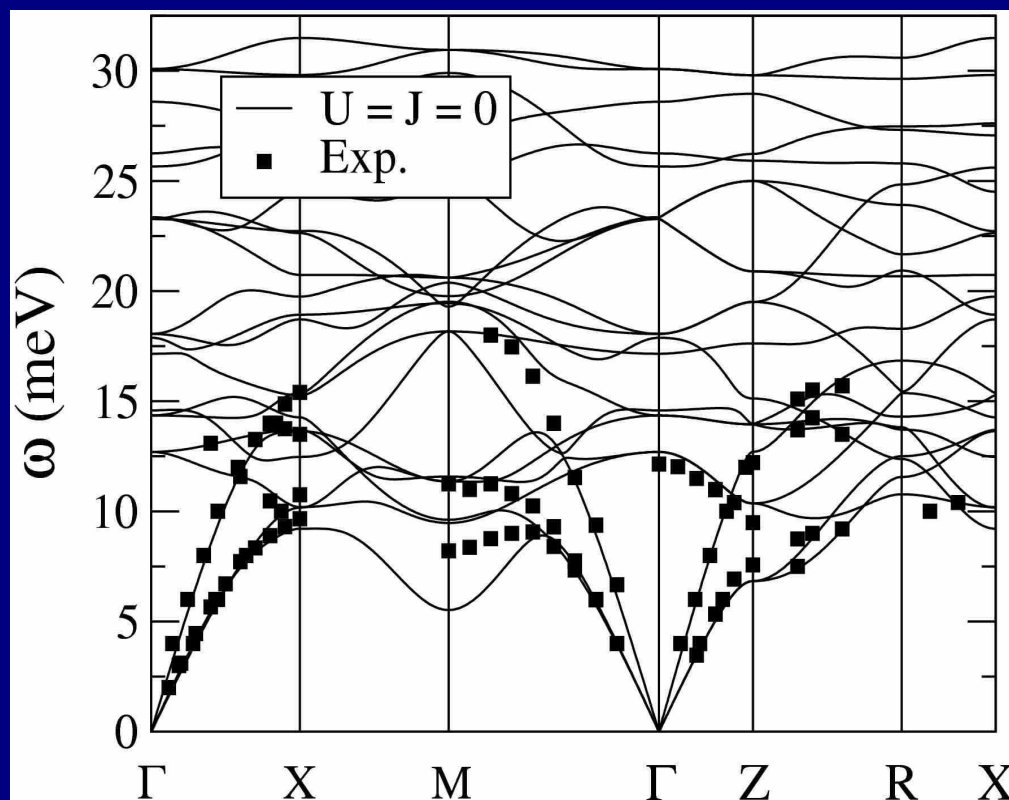
A. Szajek and J.A. Morkowski,
J. Phys. Cond. Mat. 15, L155 (2003)



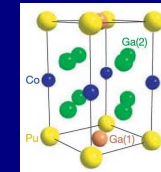
J.A. Morkowski, A. Szajek, Z. Bukowski,
C. Sułkowski, R. Troć, G. Chełkowska,
J. Magn. Magn. Mater. 272-276, 323 (2004)



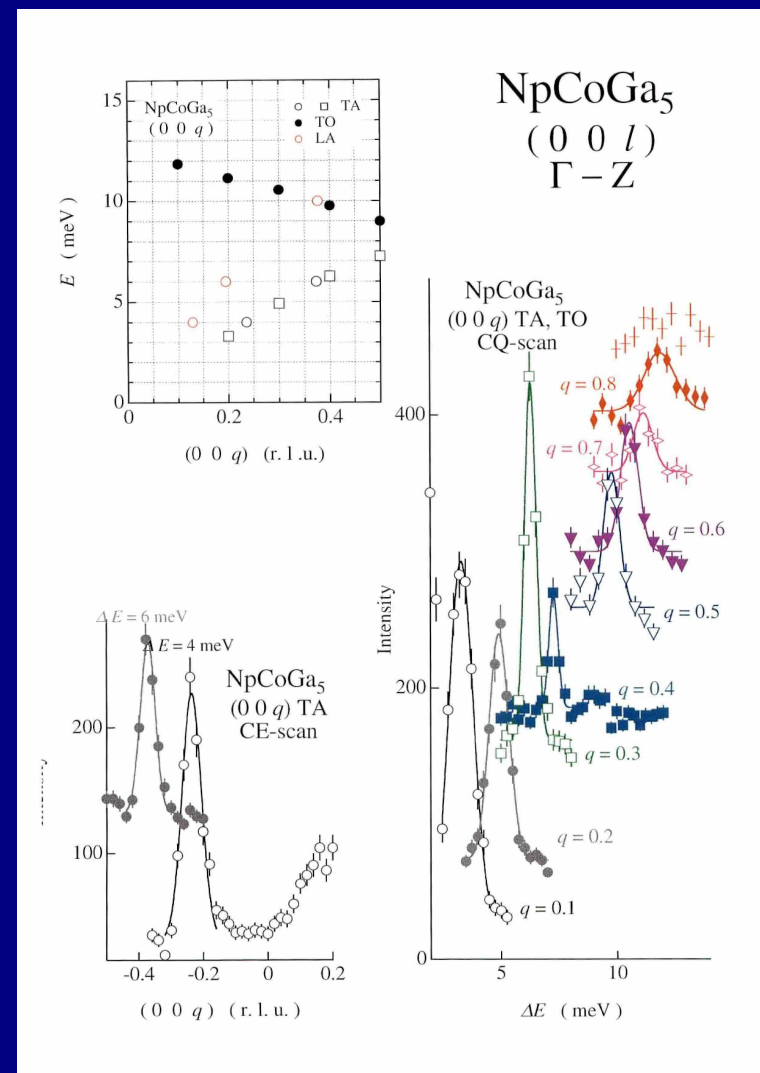
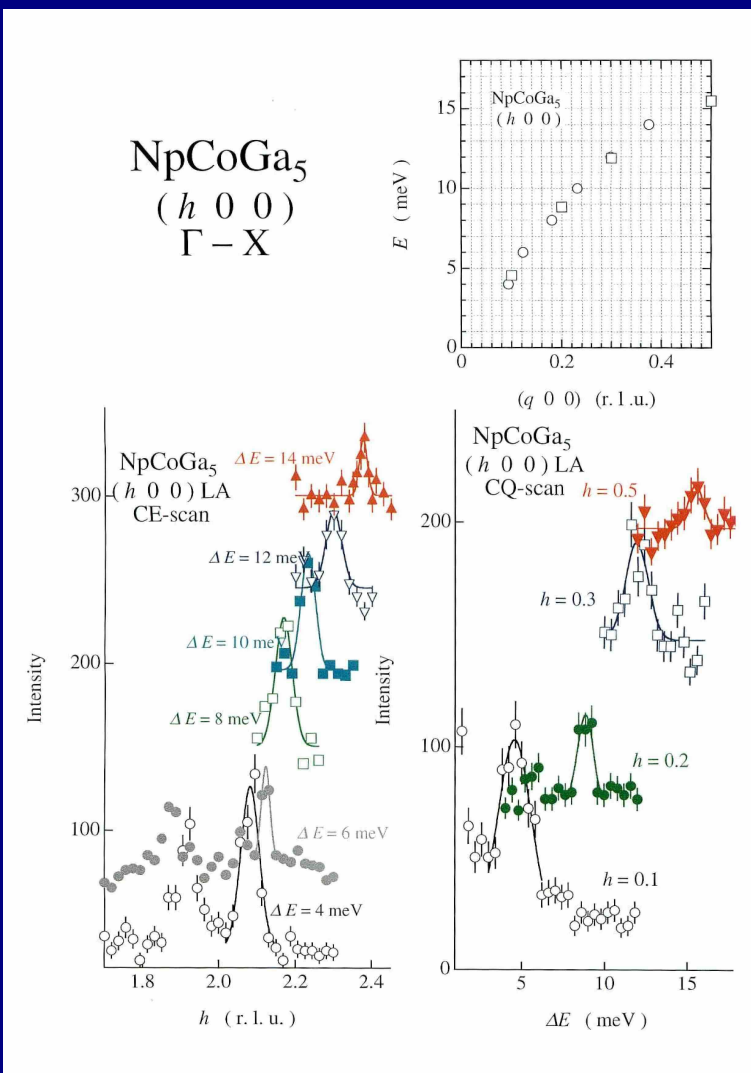
UCoGa₅ N. Metoki, INS, JAERI, Japan

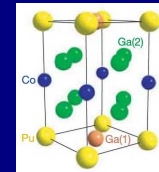


N. Metoki, K. Kaneko, S. Raymond, J.P. Sanchez, P. Piekarz, K. Parlinski, A.M. Oles, S. Ikeda, T.D. Matsuda, Y. Haga, Y. Onuki, G.H. Lander, Physica B 378-380, 1003 (2006)



NpCoGa₅





Podsumowanie

Obliczone relacje dyspersji dla PuCoGa_5 porównano z wynikami pomiarów metodą rozpraszania promieni X i neutronów.

Dobrą zgodność z eksperymentem uzyskano po uwzględnieniu lokalnych oddziaływań kulombowskich U i J dla elektronów $5f$.

Krzywe dyspersji UCoGa_5 wyznaczone dla $U=J=0$ bardzo dobrze zgadzają się z wynikami eksperymentu neutronowego.

Różnice w dynamice sieci w PuCoGa_5 i UCoGa_5 wynikają ze struktury elektronowej tych materiałów.

Dalsze obliczenia: NpCoGa_5 , UGe_2