Coupled quadrupole-phonon excitations in $CeAuAl_3$ and spin wave excitations in $MnWO_4$

B.-Q. Liu[1,2], P. Čermák[2], A. Schneidewind[2], and Sohyun Park[3]

[1]Key Laboratory of Neutron Physics, Institue of Nuclear Physics and Chemistry, CAEP, Mianyang, PR China
[2]Jülich Centre for Neutron Science (JCNS) at MLZ, Forschungszentrum Jülich GmbH, Garching, Germany
[3] Section Crystallography, Department for Earth and Environmental Sciences, Ludwig-Maximilians-Universität München, Theresienstrasse 41, 80333 Munich, Germany

Structural properties and lattice dynamics of $CeAuAl_3$

Introduction and Motivation:

√ Ce-based heavy fermion intermetallic compounds CeTX_3 (T: transition metal, X= Si, Ge, or Al)

√ Weak magnetoelastic interaction can lead to the anticrossing phenomenon in inelastic neutron scattering experiments.

√ Strong magnetoelastic interaction can lead to the formation of a bound state between phonons and crystal field (CEF) excitation, which can not be explained by a pure CEF model.

Computational method: DFT calculations have been carried out with the PAW method, GGA descriptions for the exchange-correlation functional. The cutoff energy is set as 500 eV in plane-wave basis expansion. The k-point meshes are sampled by 14 × 14 × 7 according to the Monkhorst-Pack scheme.

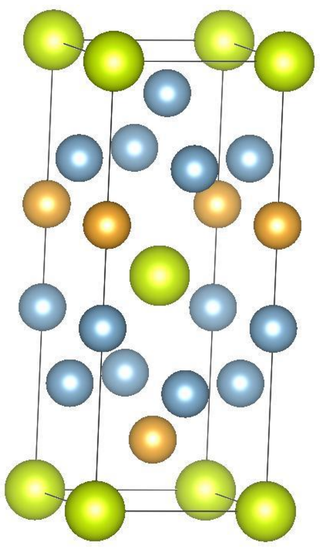

FIG. 1 Crystal structure of $CeAuAl_3$, with Ce in yellow, Au in orange, Al in blue.

The phonon calculations are performed with the finite difference method. A 2 × 2 × 2 supercell was constructed and Phonopy was used. Phonon dispersion along Γ-Z-Σ-Γ is shown in FIG. 2. The irreducible representations for the high symmetry points are: $\Gamma=4\Gamma_1+\Gamma_3+5\Gamma_5$, $Z=4\Gamma_1+\Gamma_3+5\Gamma_5$, and $\Sigma=9A'+6A''$, respectively.

Table 1. Structural parameters for $CeAuAl_3$.

	***a* (Å)**	***c* (Å)**	***c*/*a***	**V_0(Å^3)**
Expt. at 300 mK[1]	4.3105	10.7965	2.5047	200.60
Expt. at 9 K[1]	4.3172	10.8090	2.5037	201.46
Expt. [2]	4.3364	10.85	2.5021	204.03
Our DFT study	4.3354	10.8436	2.5012	203.81

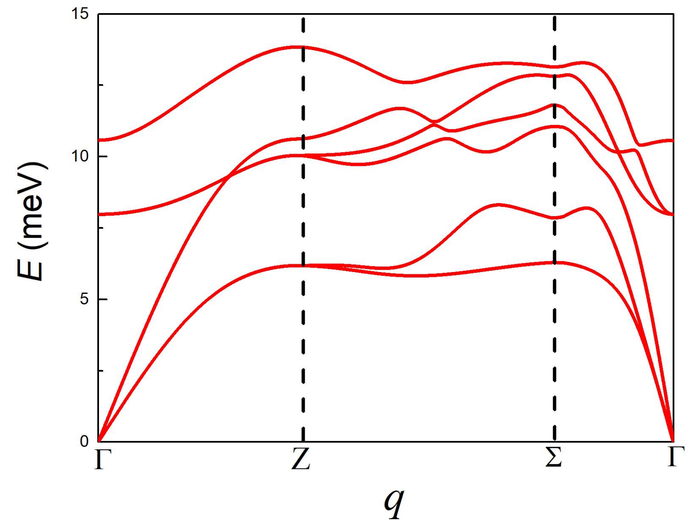

FIG. 2 Phonon dispersion for $CeAuAl_3$ along high symmetry lines Γ-Z-Σ-Γ.

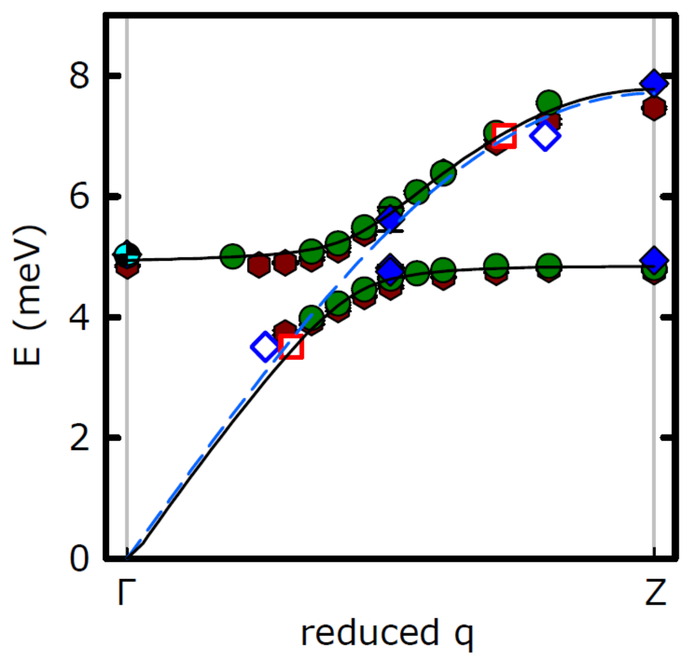

FIG. 3 Dispersion curves of the coupled excitations in $CeAuAl_3$ [3].

Summary: The magnetoelastic interaction which is not strong will lead to mixed-mode excitations of phonons and quadrupole excitations in $CeAuAl_3$.

Two spin-canting textures in the AF1 phase of multiferroic $MnWO_4$

Introduction and Motivation:

√ an exemplary prototype of magnetoelectric control, possible applications like data storage, magnetoelectric sensors

√ a promising system for the study of magnetic phase transitions and related critical phenomena

√ rich magnetic phase diagram by chemical substitutions and applying magnetic fields

√ competing long-range exchange coupling

Computational method: Total energies of both collinear (Fig. 4a) and non-collinear (Fig. 4b) AF1 models have been calculated within the PAW method, GGA descriptions for the exchange-correlation functional. The cutoff energy is 500eV in plane-wave basis expansion. A supercell with 216 atoms has been constructed, using only the Γ-point for k-point integrations.

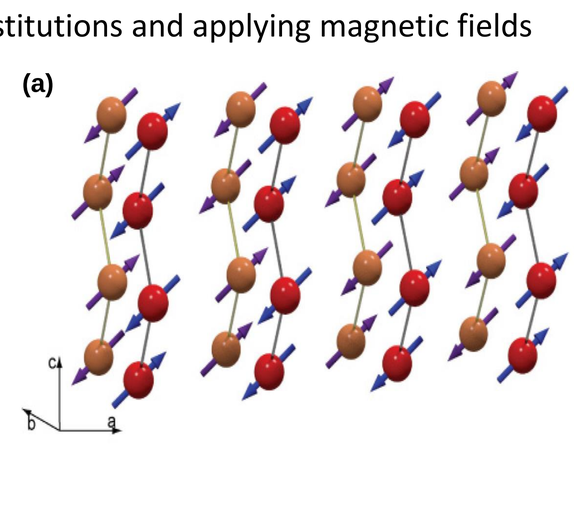

FIG. 4 The magnetic model of the AF1 phase of $MnWO_4$, (a) collinear, taken from Ref.[4], (b) non-collinear, displaying only the magnetic Mn^{2+} ions.

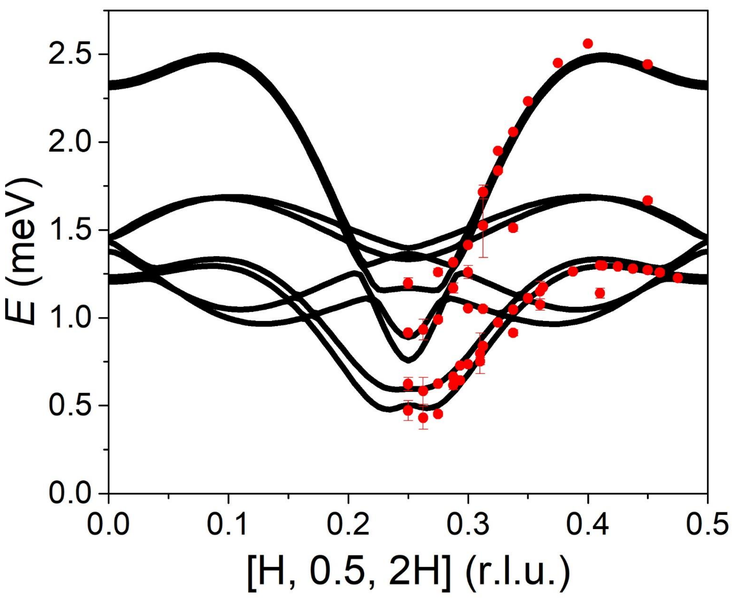

FIG. 5 The spin wave dispersion of the AF1 phase of $MnWO_4$, the red circles are experimental data taken from Ref.[5], fitted by the non-collinear model.

[1] D. T. Adroja, C. de la Fuente, A. Fraile, *et al*., PRB **91**, 134425 (2015).

[2] C. Franz, A. Senyshyn, A. Regnat, *et al*., J. Alloys & Comp. **688**, 978-986 (2016).

[3] P. Čermák, *et al.,* in preparation.

[3] F. Ye, R. S. Fishman, J. A. Fernandez-Baca, *et al*., PRB 83, 140401(R) (2011).

[4] Y. Xiao, C. M. N. Kumar, S. Nandi, *et al*., PRB 93, 214428 (2016).

Summary: The energy of the two spin-canting structure is lower than that of the collinear model, i.e., the ground state of $MnWO_4$ prefers two spin-canting textures. Besides, the lowest spin wave branch can be properly described by the spin-canting model while the collinear model with one single-ion anisotropy parameter failed.

Contact: **B.-Q. Liu**
E-mail: b.liu@fz-juelich.de
Phone: +49.89.289.54823