Abstract for an Invited Paper for the MAR10 Meeting of The American Physical Society

Interplay between phonons and magnetism in 122 ferropnictides DMITRY REZNIK, Forschungszentrum Karlsruhe: Colorado University-Boulder

The talk will focus on results of inelastic neutron and x-ray scattering measurements and density functional theory (DFT) calculations of phonon dispersions in doped and undoped CaFe₂As₂ (Ca122) and BaFe₂As₂ (Ba122). DFT predicts that the frequencies of some phonons depend strongly on the Fe moment and the relative orientation between the Fe moment and the phonon propagation vector. Thus a comparison of experimental phonon frequencies and the DFT calculations can serve as a probe of magnetism. The calculation with Fe moment fixed to zero gives correct frequencies of *most* phonons in both compounds if the calculation is constrained to the experimental crystal structure. However, in Ba122 some phonons are softer in the experiment than calculated. The agreement is improved if a large Fe magnetic moment is included into the calculation. However, this Fe moment would result in phonon peak splitting that is not observed. In addition, we found very little doping or temperature dependence of the phonons, aside from some small shifts in Ca122 across the magnetic transition. The talk will focus on how these already published results relate to out understanding of the physics of the pnictides and the coupling between phonons and magnetic fluctuations. I will also present many new unpublished results, will discuss novel recently observed magnetic modes, and will reexamine phonon peak assignements of our previous neutron scattering measurements.