

Abstract Submitted  
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**CaFe<sub>2</sub>As<sub>2</sub> Phonons via Inelastic X-ray Scattering and First Principles Calculations** STEVEN HAHN, Ames Laboratory and Iowa State University, AHMET ALATAS, BOGDAN LEU, Advanced Photon Source, Argonne National Laboratory, YONGBIN LEE, NI NI, Ames Laboratory and Iowa State University, DUCK YOUNG CHUNG, ILIYA TODOROV, Materials Science Division, Argonne National Laboratory, MERCOURI KANATZIDIS, Materials Science Division, Argonne National Laboratory and Department of Chemistry, Northwestern University, ERCAN ALP, Advanced Photon Source, Argonne National Laboratory, PAUL CANFIELD, ALAN GOLDMAN, ROBERT MCQUEENEY, BRUCE HARMON, Ames Laboratory and Iowa State University — In the iron pnictides, the sensitivity of the iron magnetic moment to the arsenic position suggests a strong relationship between phonons and magnetism. We measured the phonon dispersion of several branches in the high temperature tetragonal phase of CaFe<sub>2</sub>As<sub>2</sub> using inelastic x-ray scattering on single-crystal samples. These measurements were compared to ab-initio calculations of the phonons. Spin polarized calculations imposing the antiferromagnetic order present in the low temperature orthorhombic phase dramatically improves agreement between theory and experiment. This is discussed in terms of the strong antiferromagnetic correlations that are known to persist in the tetragonal phase.

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