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Influence of magnetism on phonons in CaFe₂As₂ as seen via inelastic x-ray scattering STEVEN HAHN, YONGBIN LEE, NI NI, PAUL CAN-FIELD, ALAN GOLDMAN, ROBERT MCQUEENEY, BRUCE HARMON, Ames Laboratory and Iowa State University, AHMET ALATAS, BOGDAN LEU, ERCAN ALP, Advanced Photon Source, Argonne National Laboratory, 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 — In the iron pnictides, the strong sensitivity of the iron magnetic moment to the arsenic position suggests a significant relationship between phonons and magnetism. We measured the phonon dispersion of several branches in the high-temperature tetragonal phase of CaFe₂As₂ 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 tetragonal phase dramatically improve 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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