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Thermoelectricity in $Ca_3Co_4O_9$: An Atomic Structure Perspective[1] T. TYSON, Z. CHEN, New Jersey Institute of Technology, J. TU, City College of New York, Q. LI, Brookhaven National Laboratory — The temperature dependent local structure about the Co sites in the misfit system referred to as $Ca_3Co_4O_9$ was examined by x-ray absorption spectroscopy. Density Functional calculations utilizing a large cell were used to obtain the optimized atomic structure. The detailed atomic structure about the Co sites was determined from the XAFS measurements. The complementary density functional computations of the structure and atomic forces provide a new 3D model of the structure and point to a unique configuration which may be the origin of the high thermoelectricity in this material.

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