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EXAFS Analysis of the Local Structure of Thermoelectric Clathrates¹ SCOTT MEDLING, MICHAEL KOZINA, FRANK BRIDGES, UC Santa Cruz — We present local structure studies of clathrates (types I, II, and VIII) using the extended X-ray absorption fine structure (EXAFS) technique. The presence of a rattler atom located in the center of one of the cages in the unit cell is believed to strongly scatter phonons and be the origin on the low thermal conductivity that makes these materials promising for thermoelectric applications. We compare a large number of similar clathrates to understand how the local structure explains the electrical and thermal conductivities. For several compounds, including Ba₈Ga₁₆Sn₃₀, EXAFS analysis shows that the local distances are different than average values found from diffraction and show greatly increased disorder compared to Ba₈Ga₁₆Ge₃₀, suggesting that the cage structure is severely distorted, scattering both phonons and electrons, and accounting for the lower thermoelectric figure of merit.

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