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Local Structure of Thermoelectric Clathrates[1] SCOTT MEDLING, FRANK BRIDGES, University of California, Santa Cruz, TOSHIRO TAKABATAKE, Hiroshima Univeristy — We present local structure results from extended X-ray absorption fine structure (EXAFS) analysis of two new kinds of clathrates: type I clathrates with a light 'rattler' atom and type VIII clathrates. The rattler atom is extremely important for the thermoelectric properties as it is what strongly scatters phonons and lowers the thermal conductivity without affecting the electrical conductivity. In most thermoelectric clathrates, the rattler atom is a heavy atom, typically Ba or Eu, and such type I clathrates have been discussed extensively in the literature; a smaller rattler atom such as K results in more free space inside the cage. Type VIII clathrates have the same chemical formula as type I clathrates, but have a different, more distorted, cage structure resulting in differing electronic properties. Recent studies indicate a thermoelectric figure of merit at least as high as 1.2 at 400 K is attainable. For both kinds of clathrates, we collect and analyze temperature-dependent data over the range 10-300 K and compare the results with our models.

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Scott Medling
University of California, Santa Cruz

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