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Enhanced Thermoelectric and Mechanical Properties of $Cu_{1.8}S_{1-x}P_x$ Bulks Mediated by Mixed Phase Engineering

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Part 1. Supplementary Data and Diagrams

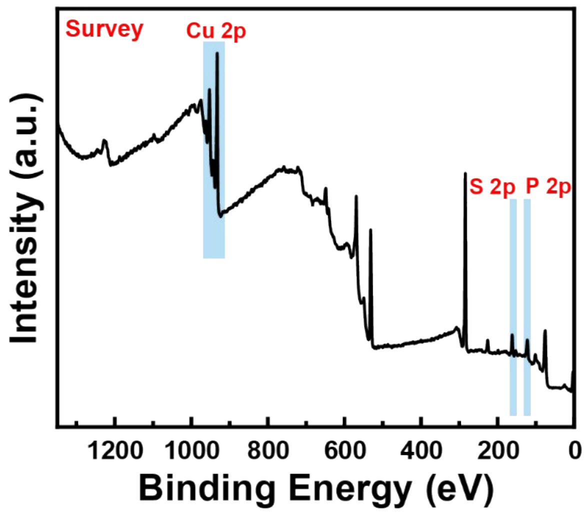

Fig. S1 XPS survey scan of the $Cu_{1.8}S_{0.97}P_{0.03}$.

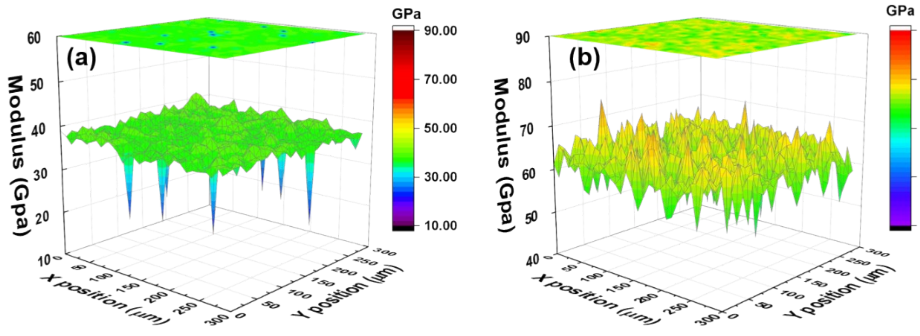

Fig. S2. Mechanics properties of $Cu_{1.8}S_{1-x}P_x$ bulk samples. 3D cloud image of modulus for a) pure $Cu_{1.8}S$, b) $Cu_{1.8}S_{0.97}P_{0.03}$.

Part 2. Single Parabolic Band (SPB) modeling

The $Cu_{1.8}S$, as a kind of degenerate semiconductor, can be analyzed by the Single Parabolic Band (SPB) Model with relaxation time approximation. The Seebeck coefficient can be expressed as:

$$S = \frac{k_B}{e}\left[\frac{\left(\frac{5}{2}+\lambda\right)F_{\lambda+\frac{3}{2}}}{\left(\frac{3}{2}+\lambda\right)F_{\lambda+\frac{1}{2}}} - \eta\right] \tag{1}$$

The charge carrier concentration can be expressed as:

$$n_H = 4\pi\left(\frac{2m^* k_B T}{h^2}\right)^{3/2} F_{1/2} \tag{2}$$

The effective mass (m*) can be expressed as:

$$m^* = \frac{h^2}{2k_B T}\left[\frac{n}{4\pi F_{\frac{1}{2}}(\eta)}\right]^{\frac{2}{3}} \tag{3}$$

The Fermi integral can be expressed as:

$$F_i(\eta) = \int_0^\infty \frac{x^i dx}{1 + exp(x-\eta)} \tag{4}$$

where η is the simple Fermi energy, $F_i(\eta)$ is the i-th Fermi integral, k_B is the Boltzmann constant, h is the Planck constant, and r is the scattering factor usually to be—0.5 meaning the main scattering mechanism is acoustic phonon scattering.