

Supporting information

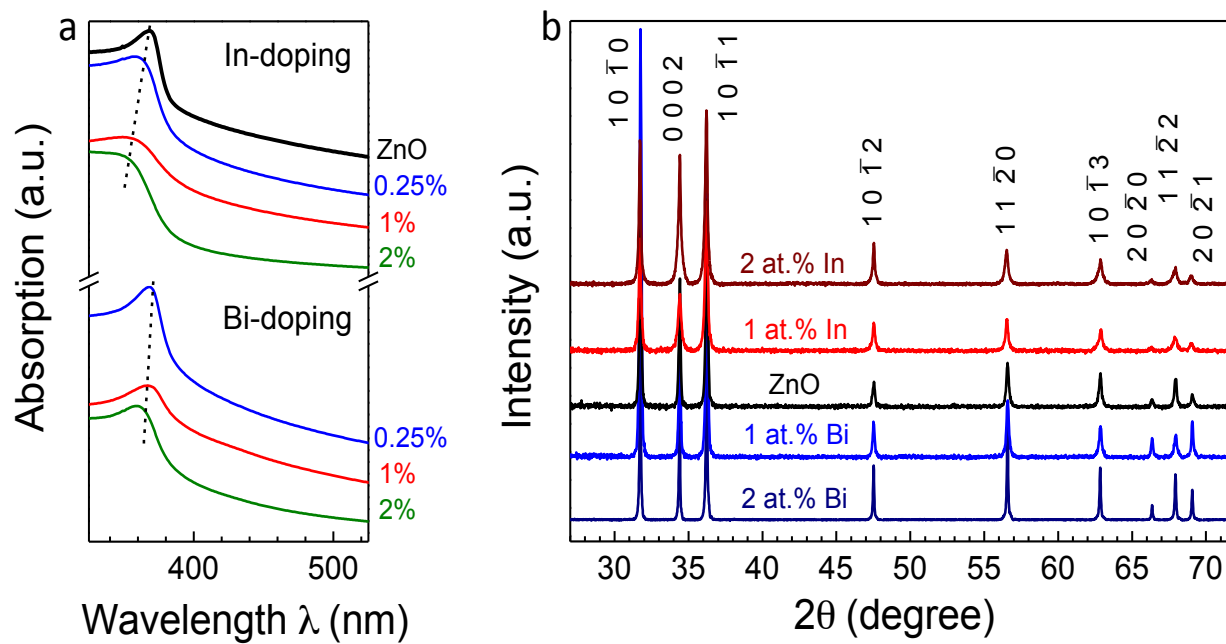


Fig. S1. (a) Optical absorption spectra from as-synthesized In- and Bi-doped ZnO nanocrystal solutions showing absorption band edge shifts as a function of the doping level. (b) X-ray diffractograms from In- and Bi-doped ZnO nanobulk pellets.

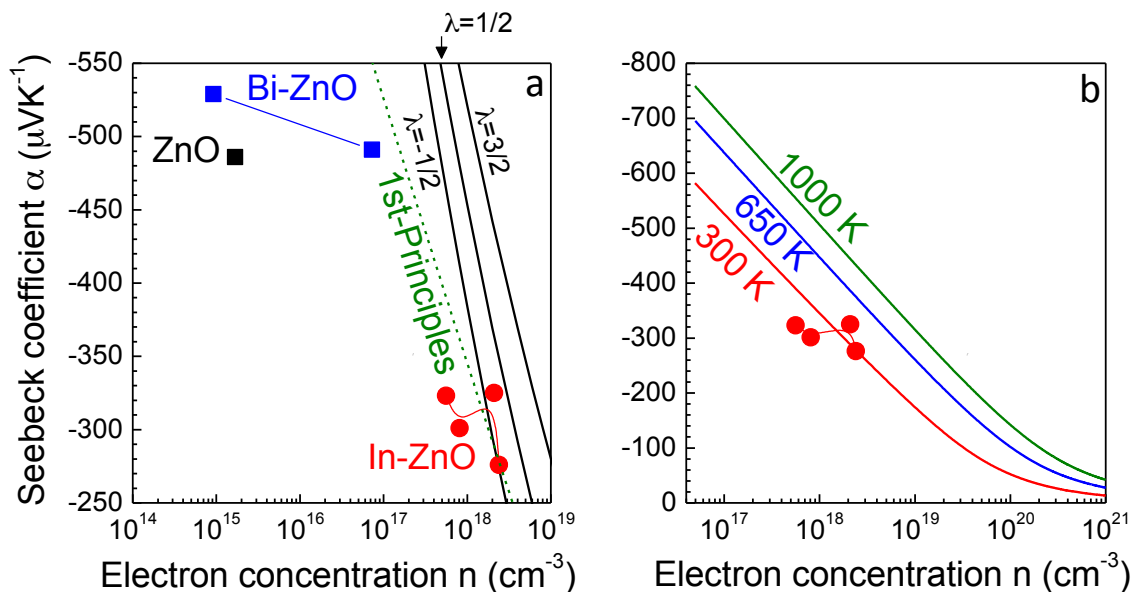


Fig. S2. (a) Room-temperature Seebeck coefficient $\alpha_{300\text{K}}$ plotted as a function of electron concentration. The solid lines correspond to model fits with $\lambda = 1/2$, $3/2$ and $-1/2$, denoting electron scattering from optical phonons, ionized impurities, and acoustic phonons, respectively and the green dashed line represents the first principles model^{R1}. (b) Direction-averaged Seebeck coefficient as a function of doping at different temperatures from first principles calculations carried out within the constant scattering time approximation^{R1}. The red circles are experimental data from In-doped ZnO at 300 K.

R1: K. P. Ong, D. J. Singh, P. Wu, *Phys. Rev. B.* **2011**, 83, 115110.

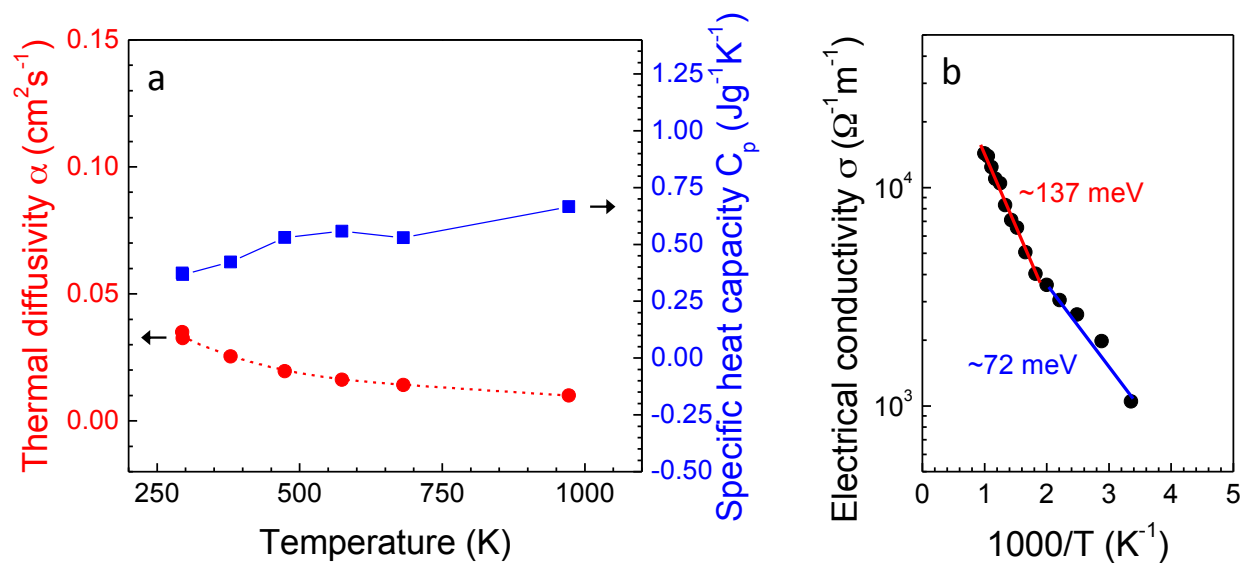


Fig. S3. (a) Temperature-dependent thermal diffusivity and specific heat capacity, and (b) electrical conductivity versus temperature showing the two different activation energy regimes indicating the donor states for 0.5 at.% In-doped nanobulk ZnO.