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Phonon Engineering of ZnO nanowires with controlled chemical doping JAIME BOHORQUEZ-BALLEN, THUSHARI JAYASEKERA, Southern Illinois University Carbondale — Using the first principles density functional theory (DFT) calculations, we have investigated electronic and dynamical properties of ZnO nanowires in [001] direction with different diameters in the presence of impurities such as Mg, Al, and Ga. As the impurity concentration is varied, electrical and thermal conductivities of nanowires change. In this way, nanowires can be engineered to reduce the thermal transport, such that their thermoelectric properties can be enhanced.

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