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Structure and Properties of a Metallic Polar Ruthenate Oxide¹ DANILO PUGGIONI, JAMES RONDINELLI, Drexel Univ — Using first-principles density functional theory calculations, we predict a polar-noncentrosymmetric (pNCS) ruthenate exhibiting robust metallicity. We describe a weak coupling ansatz which accounts for the scarcity of noncentrosymmetric metal (NCS-M). We show in this artificial ruthenate that the apparent incompatibility between acentricity and metallicity is circumvented because the polar distortion is largely decoupled from the electronic structure at the Fermi level. Moreover, we discuss the thermopower response showing that this material owns an anomalously anisotropy at 300 K which is comparable to that of YBa₂Cu₃O_{7- δ}, owing to the polar axis. Our work suggests it is possible to design thermopower anisotropy in noncentrosymmetric conductors for ultrafast-thermoelectric devices.

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