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First-principles prediction of a native ferroelectric metal[1] JORGE INIGUEZ, Luxembourg Institute of Standards and Technology, ALESSIO FILIPPETTI, CNR-IOM SLACS Cagliari, VINCENZO FIORENTINI, Universit di Cagliari and CNR-IOM SLACS Cagliari, FRANCESCO RICCI, Universit di Cagliari, PIETRO DELUGAS, Istituto Italiano di Tecnologia IIT — The possibility that metals may support ferroelectricity is an intriguing open issue. Over the years, various compounds have been referred to as ferroelectric metals, including non-centrosymmetric metals as well as ferroelectrics whose polar distortion survives moderate metallicity induced by doping or proximity. Yet, we think none of these systems embodies a truly ferroelectric metal with native switchable polarization and native metallicity coexisting in a single phase. Here we report a first-principles prediction of such a material. We show that the layered perovskite Bi5Ti5O17 has a non-zero density of states at the Fermi level and metal-like conductivity, as well as a spontaneous polarization in zero field. Further, we predict that the polarization of Bi5Ti5O17 is switchable both in principle (the material complies with the sufficient symmetry requirements) and in practice (in spite of being a metal, Bi5Ti5O17 can sustain a sizable potential drop along the polar direction, as needed to revert its polarization by application of an electric bias). Our results also reveal striking behaviors – such as the self screening mechanism at work in thin Bi5Ti5O17 layers – emerging from the intimate interplay between polar distortions and free carriers in such an exotic material.

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