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Weyl Semimetal Phase in Noncentrosymmetric Transition-Metal Monophosphides

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Based on first-principle calculations, we show that a family of nonmagnetic materials including TaAs, TaP, NbAs, and NbP are Weyl semimetals (WSM) without inversion centers. We find twelve pairs of Weyl points in the whole Brillouin zone (BZ) for each of them. In the absence of spin-orbit coupling (SOC), band inversions in mirror-invariant planes lead to gapless nodal rings in the energy-momentum dispersion. The strong SOC in these materials then opens full gaps in the mirror planes, generating nonzero mirror Chern numbers and Weyl points off the mirror planes. The transport properties obtained by the Boltzmann equation combined with the semiclassical treatments of the unique electronic structure in these materials will also be discussed in comparison with the most recent experimental data.