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Large Fermi-Energy Shift and Suppression of Trivial Surface States in NbP Weyl Semimetal Thin Films

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Fig. S1: Height profile across the surface of NbP, taken from an overview scanning tunneling microscopy image (Figure 1a – marked with an arrow). Atomically-flat terraces, corresponding to each Nb-P layer (2.8 Å) of the NbP structure, can be well distinguished. A NbP unit cell in (001) direction, composed of 4 Nb-P individual layers, is drawn as guide to the eye.
Fig. S2: Band structure of the P (√2 × √2) reconstructed NbP surface. a) The relationship between the 1st Brillouin Zones for the primitive cell (blue) and √2 × √2 supercell (black). The AA’ line in the Brillouin Zone of the primitive cell corresponds to a line cut across a pair of Weyl points. b) Surface band structure for the supercell along the k paths as shown in a), showing topological surface states (TPSS1) at the positions where the Weyl points (along AA’) are expected. Note that the Σ1 (Σ4) is close to the other pair of Weyl points on k_y0 axis of the primitive cell Brillouin Zone, which results in the states near the Fermi-level Σ1 (Σ4) and a linear dispersion (TPSS2). c) Surface-projected constant-energy contours of the √2 × √2 supercell at different binding energies (in eV). In both b) and c), the Fermi level is set as the energy zero.
Figure S3: Electronic structure upon Se-doping in NbP (a-c) and TaP (b-d) thin films.

Constant-energy contours at the Fermi-energy show very similar electronic pockets following four-fold symmetry for NbP (a) and TaP (d) thin film surfaces. The dispersion cuts along Γ→X and M→X directions evidence a Fermi-level shift of around 0.3eV with respect to the intrinsic chemical potential both for NbP (b,c) and TaP (e,f). These results highlight the reproducibility of the Se-doping strategy to account for Fermi-level engineering on the Weyl monopnictide family.