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Topological Dirac semimetallic phase in transition metal compounds PENG-JEN CHEN, WAN-JU LI, TING-KUO LEE, Academia Sinica — It is known that the transition metal monoarsenides/phosphides (TaAs, TaP, NbAs, and NbP) are Weyl semimetals that can host the long-sought Majorana fermions. Motivated by these exciting findings, we find that some of their allotropes reveal three-dimensional Dirac points. Based on the classification of three-dimensional topological Dirac semimetals proposed by Yang and Nagaosa (Nat. Commun. **5**, 4898 (2014)), the nontrivial topology is confirmed by computing the corresponding topological invariant. That is, we propose a new family of topological Dirac semimetals other than Na₃Bi and Cd₃As₂. Besides, our results also indicate that the crystal symmetry plays an important role in determining the properties of the Dirac states and topological phase.

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