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Cubic Dirac fermions in quasi-one-dimensional transition-metal chalcogenide semimetals immune to Peierls distortion[1] QIHANG LIU, ALEX ZUNGER, University of Colorado, Boulder — A Cubic Dirac Fermion in condensed-matter physics refers to a band crossing in periodic solids that has 4-fold degeneracy with cubic dispersions in certain directions. Such a crystalline symmetry induced fermion is composed of 6 Weyl fermions where 3 have left-handed and 3 have right-handed chirality, and constitutes one of the "new fermions" that have no counterpart in high-energy physics. However, no prediction has yet pointed to a plausible example of a material candidate hosting such a cubically-dispersed Dirac semimetal (CDSM). Here we establish the design principles for CDSM finding that only 2 out of 230 space groups possess the required symmetry elements. Adding the required band occupancy criteria, we conduct a material search using density functional band theory identifying a group of quasi-one-dimensional molybdenum chalcogenide compounds $A(MoX)_3$ (A = Na, K, Rb, In, Tl; X = S, Se, Te) with space group $P6_3/m$ as ideal CDSM candidates. Studying the stability of the $A(MoX)_3$ family towards a Peierls distortion reveals a few candidates such as $Rb(MoTe)_3$ and $Tl(MoTe)_3$ that are resilliant to Peierls distortion, thus retaining the metallic character.

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