Pairwise creation/annihilation of Weyl nodes by tunable structural phase transition in $MoTe_2$

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Abstract

$MoTe_2$ is a layered material with rich physics arising from structural and electronic phase competition. We investigate the energetics of the possible structural phase transitions and compute the potential energy surface profile of $MoTe_2$. We further explore the possibility of controlling the dynamics of Weyl fermions in noncentrosymmetric T_d-$MoTe_2$. Our first-principles calculations reveal that one can systematically tune the location and chirality of Weyl nodes by exploiting the connection between polar distortions and spin-orbit coupling effects in T_d-$MoTe_2$. We find that a total 6 pairs of Weyl nodes exist in the Brillouin zone of T_d-$MoTe_2$, and further demonstrate that one can mutually create/annihilate pairs of Weyl nodes by tuning the magnitude of the inversion symmetry breaking parameter.