

Abstract Template

Spontaneous inversion symmetry breaking and emergence of Berry curvature and orbital magnetization in topological ZrTe₅ films

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ZrTe₅ has recently attracted much attention due to the observation of intriguing nonreciprocal transport responses which necessitate the lack of inversion symmetry (\mathcal{I}). However, there has been debate on the exact \mathcal{I} -asymmetric structure and the underlying \mathcal{I} -breaking mechanism. Here, we report a spontaneous \mathcal{I} breaking in ZrTe₅ films, which initiates from interlayer sliding and is stabilized by subtle intralayer distortion. Moreover, we predict significant nonlinear anomalous Hall effect (NAHE) and kinetic magnetoelectric effect (KME), which are attributed to the emergence of Berry curvature and orbital magnetization in the absence of \mathcal{I} symmetry. We also explicitly manifest the direct coupling between sliding ferroelectricity, NAHE, and KME based on a sliding-dependent $k \cdot p$ model. By studying the subsurface sliding in ZrTe₅ multilayers, we speculate that surface nonlinear Hall current and magnetization would emerge on the natural cleavage surface. Our findings elucidate the sliding-induced \mathcal{I} -broken mechanism in ZrTe₅ films and open new avenues for tuning nonreciprocal transport properties in van der Waals layered materials.