Photo-induced electronic and spin topological phases in monolayer single-element ferroelectrics

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Abstract

Monolayer group-V materials exhibit rich physics such as single-element ferroelectricity, nontrivial topology, varied spin-orbit coupling, and light-induced structural dynamics. We show with *ab initio* calculations that light can induce hidden transient phases in both the ferroelectric and paraelectric monolayers. We illustrate the nontrivial topological character of these system by using the recently introduced idea of spin bands and spin-resolved Wilson loops, and show that the topology changes via the closing of the respective band gaps in the presence or absence of photo-induced structural phase transitions. The evolution of topological edge states is also discussed. Our study provides multiple strategies to tailor electronic and spin topology via ultrafast control of photo-excited carrier and structural dynamics.

References

[1] B Peng, GF Lange, D Bennett, K Wang, RJ Slager and B Monserrat. *Physical Review Letters*, in press (2024)

Figures

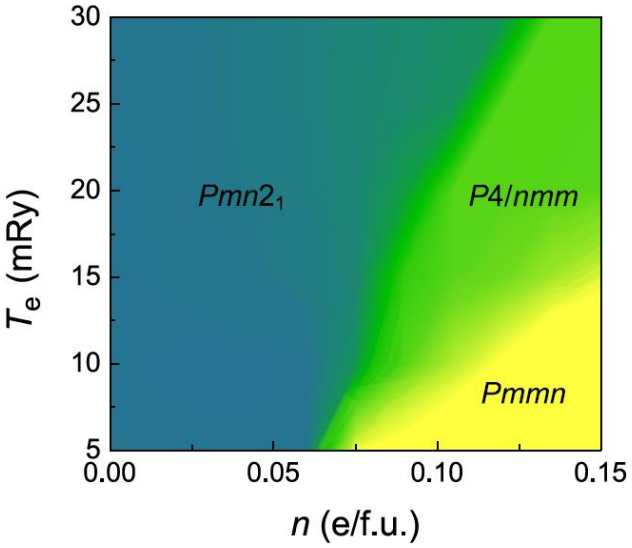

Figure 1: Phase diagram for monolayer ferroelectric $Pmn2_1$ Bi as a function of photoexcited carrier density n in electron-hole pairs per unit cell (e/f.u.) and electronic temperature T_e in mRy.

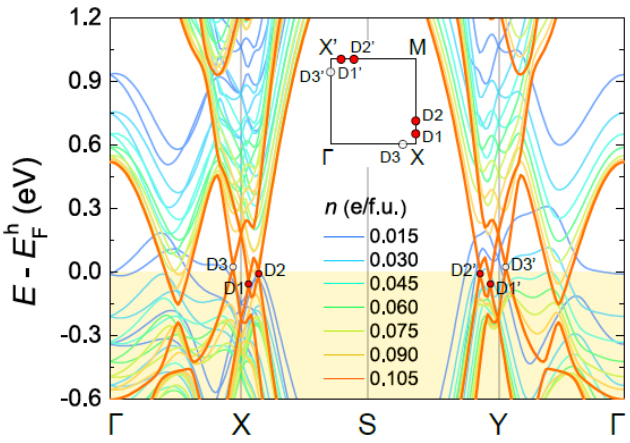

Figure 2: Band structure of $Pmn2_1$ Bi as a function of n for T_e = 20 mRy, with the quasi-Fermi level for holes E_F^h set to zero. At n = 0.105 e/f.u., the doubled quantum spin Hall insulator becomes a 2D Dirac semimetal with space group $P4/nmm$. The inset shows the 2D Brillouin zone with the Dirac points denoted as D.